Electronic Structure and Theoretical Modeling of UV-Vis-NIR spectra of Ferrocene-Containing Tetraazaporphyrins

A Thesis Submitted to the Faculty of the University of Minnesota by

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Advised by Dr. Viktor Nemykin

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Abstract

The UV-Vis-NIR spectra of two ferrocene substituted tetraazaporphyrins were analyzed by use of time dependent density functional theory (TDDFT) and polarized continuum model TDDFT (PCM-TDDFT) methods. The TDDFT and PCM-TDDFT calculations were done using four different exchange-correlation functionals (BPW91, BP86, B3LYP, PBE1PBE) with varying amounts of Hartree-Fock exchange included in the functional to find the best agreement between theory and experiment. Once the best agreement was found by comparing experimental spectrum to the PCM-TDDFT calculations, using the B3LYP functional, further calculations were carried out with this functional to assign the electronic transitions that made up the UV-Vis-NIR spectrum and generate the contours of the corresponding molecular orbitals involved. Once assigned, transitions toward the near-IR end of the spectrum (Identified by Region 1; see Figure 12) were found to be predominately metal-to-ligand charge transfer transitions (MLCT) between the iron atoms of the ferrocene substituents and the π* system of the tetraazaporphyrin ring. Transitions toward the UV end of the spectrum (Identified by Region 4; see Figure 12) were found to be predominately π→π* transitions of the tetraazaporphyrin ring. If was also found that the major transitions are fairly mixed in character due to mixed nature of the molecular orbitals involved, containing varying percentages of both tetraazaporphyrin and ferrocene character.

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Introduction:

With a potential energy crisis arising in the near future, renewable energy is currently a popular focus for research groups[1-5]. With the sun being a powerful source of free energy, much of this research is devoted to finding cheap and efficient ways to harvest solar energy with cells utilizing the photovoltaic effect [6-10]. There are many different types of solar cells currently being

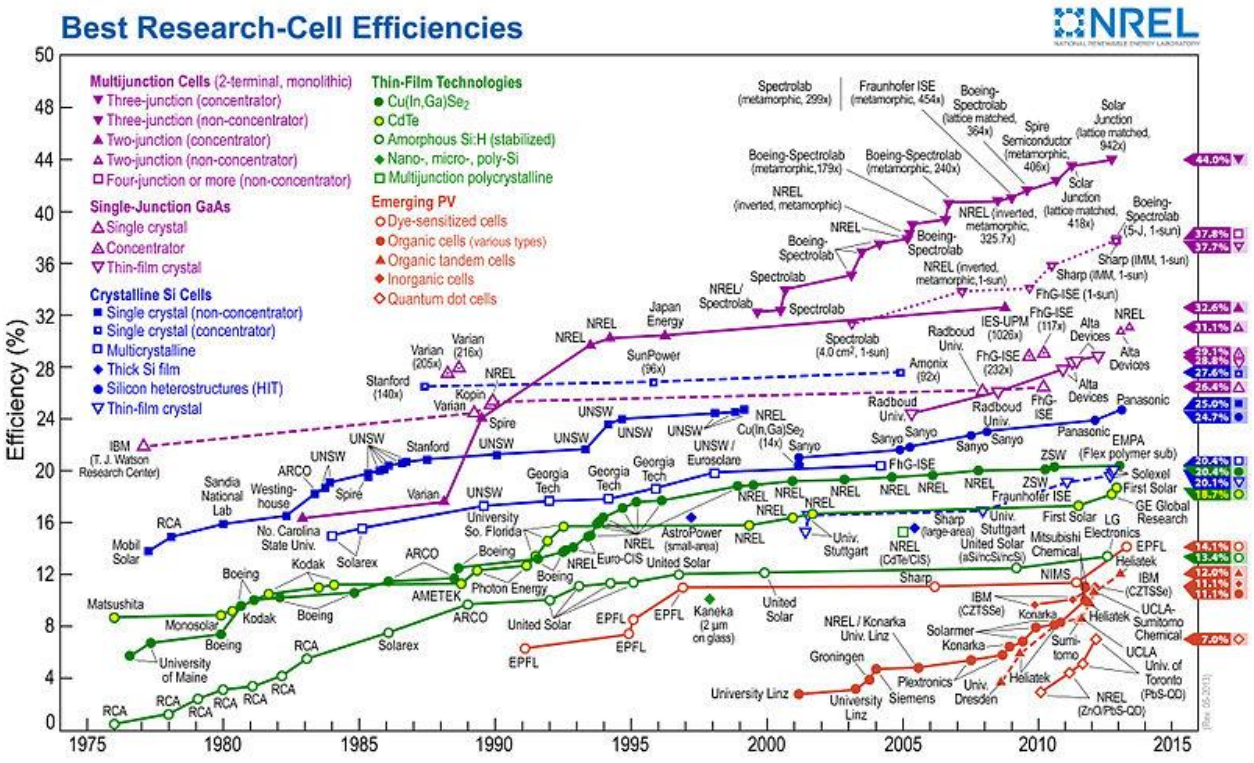


Figure 1. A plot showing major types of solar cells and their efficiency over time. Each point is labeled with the institution or research group associated with that particular advance in efficiency [11].

researched and produced all with varying levels of efficiency and cost/benefits (Figure 1). Currently, the most recognizable form of solar cells are those that are made from amorphous silicon. These amorphous silicon solar cells are cheap, often found powering

small devices such as calculators, but are relatively inefficient. There has also been little achieved to reduce cost or increase efficiency in recent years[12]. There is another type of cell that utilizes single crystal silicon that greatly improves efficiency, but is much more expensive [13]. Also, the manufacturing of silicon based cells can have environmentally toxic byproducts[14]. One theoretically very efficient type of thin film cell is a cell that uses inorganic nitrides (a popular compound of this class is indium gallium nitride, InGaN) [15] as components of a multi-junction solar cell. These types of cells can be engineered by tuning the band gap to provide a good match to the solar spectrum[16]. These alloys can absorb from the infrared region, with higher indium percentage[17, 18], to the ultraviolet region, with high gallium percentage[17, 19]. However, these types of compounds are expensive and can potentially be toxic. Current research suggests that thin film solar cells have the potential to achieve an acceptable compromise between efficiency and cost. Within the realm of thin film solar cells, there are again many different types, categorized by the compound used for the solar "antenna". An emerging type of solar cell that has the potential to be both efficient and cheap, and will also be the focus of this study, is the dye-sensitized solar cell (DSSC).[20-23] These differ from traditional solar cells in that the dye only absorbs light, while an included semiconductor acts as a charge carrier.[24] The dyes that are used as antenna compounds in DSSC are often relatively inexpensive to synthesize, so much so that there are do it yourself kits available to the general public that contain the dye and all the necessary materials for a complete and functional DSSC.

The actual technology of DSSC is relatively new, emerging roughly two decades ago. The use of porphyrins (and related compounds such as phthalocyanines) emerged

soon after, but only recently has been seen as attractive due to recent advances in solar light conversion efficiency, or the ability of a compound or cell to convert harvested solar energy into electricity, of the compounds.

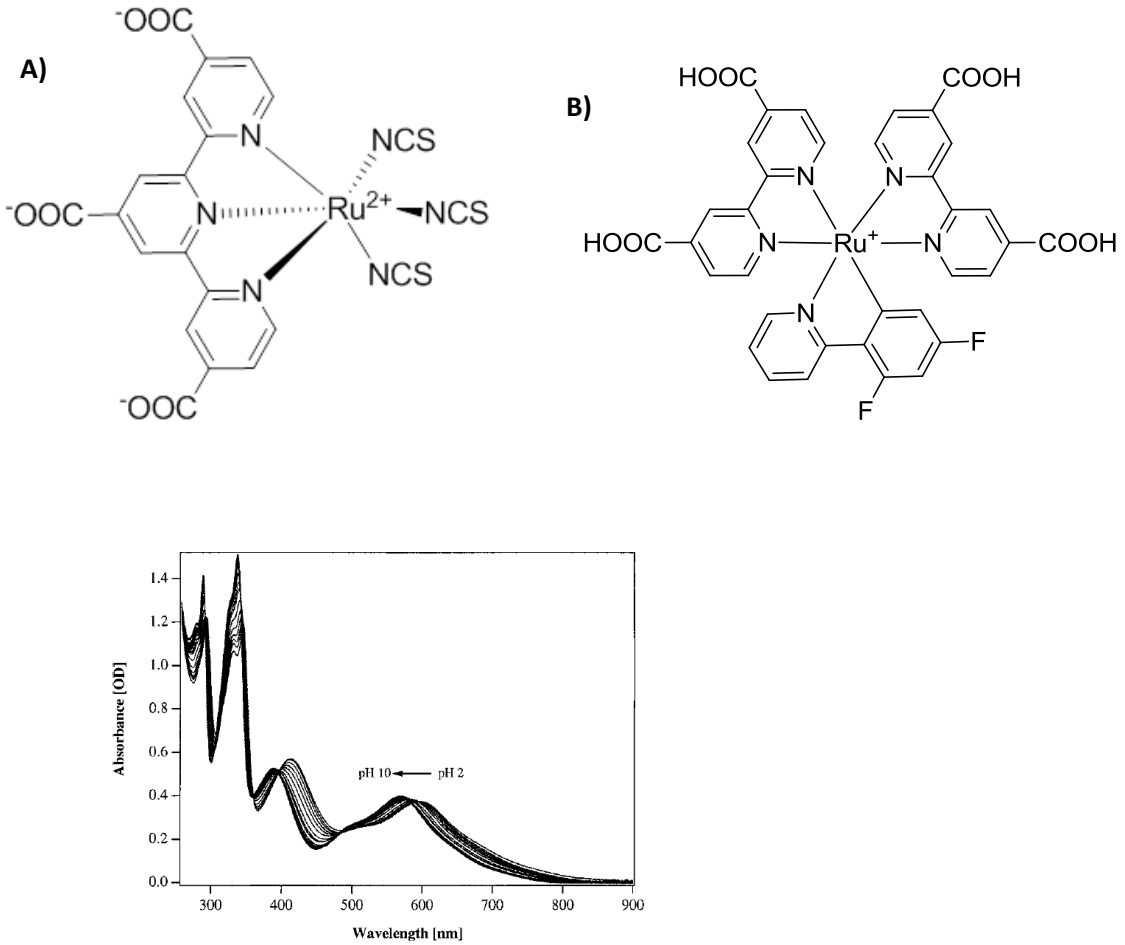


Figure 2. Top:A) [Ru(4,4',4''-tricarboxy-2,2':6',2''-terpyridine)(NCS)$_3$]$^-$, Ruthenium terpyridine dye, also referred to as "black dye". B) bis(4,4'-dicarboxy-2,2'-bipyridine)-2-(2,4-difluorophenyl) pyridine ruthenium(II) Bottom: Absorbance spectrum of black dye with varying pH [25]. Plot reprinted with permission from Nazeeruddin, M; et al. Engineering of Efficient Panchromatic Sensitizers for Nanocrystalline TiO2-Based Solar Cells. J. Am. Chem. Soc. 2001, 123, 1613-1624. © 2001, American Chemical Society

The frontier compound used for DSSC was a ruthenium terpyridine dye (referred to in literature as "black dye" and shown in Figure 2 Compound A) originally synthesized by Grätzel and co-workers. This class of dyes rely on charge transfer (Ru to terpyridine

ligand, with a carboxylic acid group acting as the anchor to the TiO_2 electrode)[26] transitions to achieve electron transfer in DSSC (diagram of process shown in Figure 3)[27]. The dye, along with an electrolyte, typically iodine/triiodide couple for Ru dyes, is placed between two electrodes, typically TiO_2 for the cathode and gold for the anode.[28, 29] In the case of ruthenium dyes, the UV-Vis spectrum is comprised of both metal to ligand charge transfer and $\pi \rightarrow \pi^*$ transitions, however only the MLCT transitions occur in the visible range (~400-700 nm) of the solar spectrum. Once excited, the dye can either relax to the original ground state, or inject and electron into the cathode surface. If an electron is injected into the cathode, the dye itself is no longer a neutral species, with the ruthenium atom being oxidized from +2 to a +3 oxidation state. Once the injected electron travels through the cell, it exits the anode and reduces iodine to triiodide. The triiodide then reduces the ruthenium +3 back to +2 to return the dye to the original oxidation state (Figure 3).

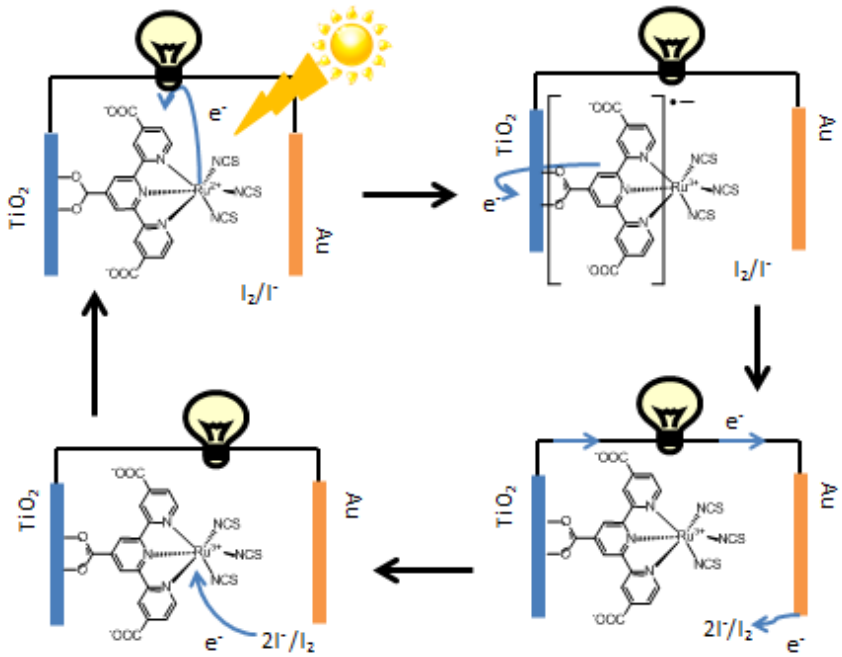


Figure 3. Typical dye sensitized solar cell based on ruthenium "black dye" with electron flow shown.

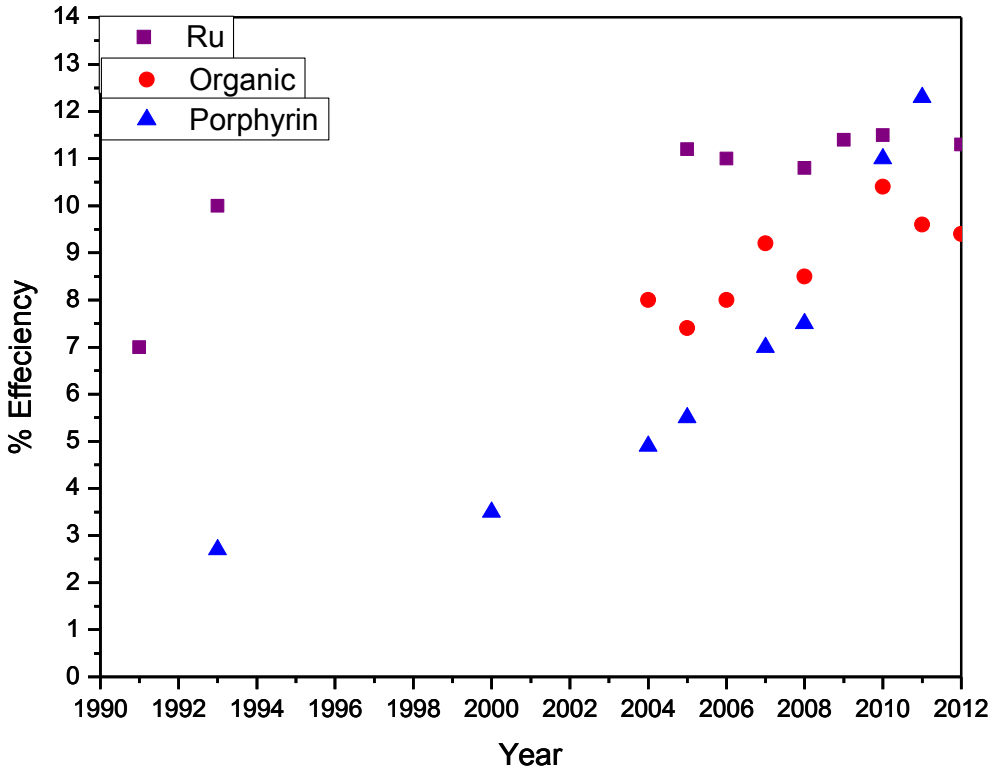
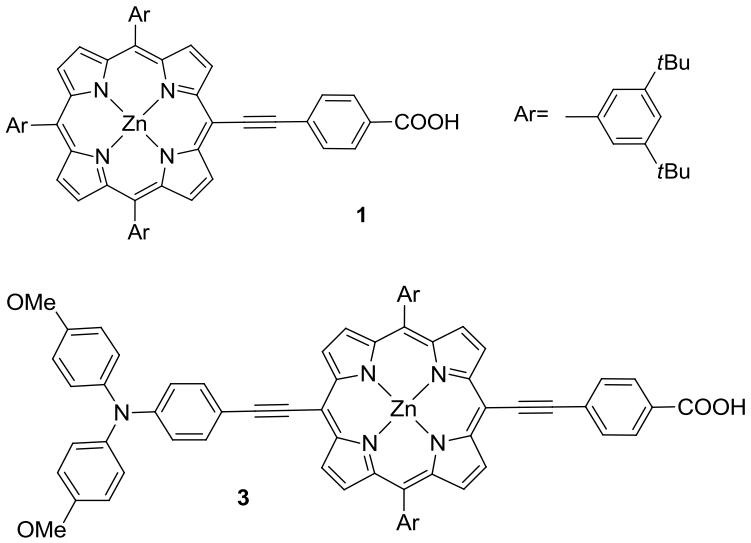


Figure 4. Solar power energy conversion of dyes used in DSSC over time shown. Efficiency of ruthenium dyes, and to an extent organic dyes, have stayed fairly level in recent years, compared to Porphyrins which have been achieving great increases in solar efficiency[31]. Plot adapted from Figure 1 in Reference 30 by Diau and Li.

However, frontier ruthenium dye compounds (such as Compound A shown in Figure 2) had a solar efficiency rating of just under 10%. The current record for solar efficiency of ruthenium dyes (Figure 2 Compound B) is 11.3%[32]. This makes the solar efficiency increase over the past two decades of about 2%, which marks relatively small gain for fairly long period of time (as shown in Figure 4). This trend is also apparent in the research of organic dyes, which are also beginning to show smaller gains in solar

efficiency[33]. Ruthenium as an element is rather limited in abundance and thus can be quite expensive, making any compound derived from the element also quite expensive[34]. Also, as shown by the previously mentioned UV-Vis-NIR spectra of black dye, ruthenium based dyes do not absorb solar light after about 700 nm and approaching the NIR range[35]. The solar spectrum is still quite active in the NIR range after 700 nm, leading to a sizable portion of the solar spectrum that is not absorbed by Ru-based dyes. This has led to other types of dyes being researched for possible use in DSSC in the search for cheaper and more solar efficient compounds. This is the reason that porphyrin dyes and similar compounds have been researched for use in DSSC (a series of which are shown in Figure 5). Although the current record for solar efficiency of porphyrin compounds is 12.3% (Compound 5 in Figure 5), the overall solar efficiency porphyrin compounds has increased rapidly over the past few years, rising from an initial low of 2% to the current 12% over the same amount of time as ruthenium dyes have only increased about 2%.



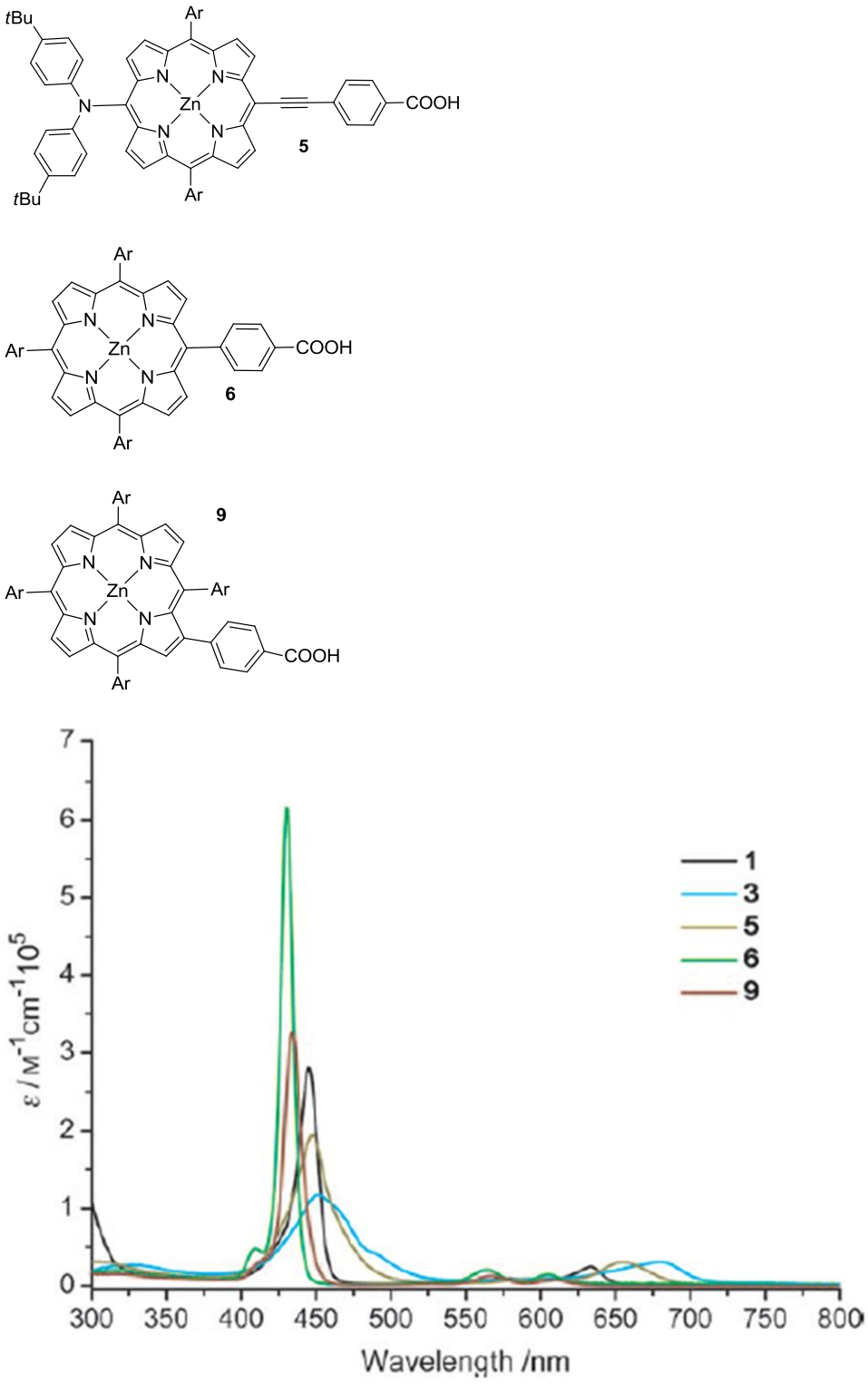
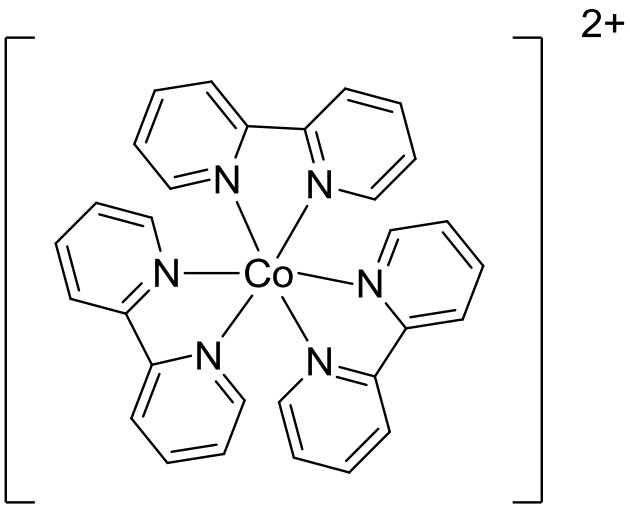


Figure 5. A series of substituted porphyrins for potential use in DSSC and their absorbance spectra.[36] *Plot reprinted from Lee, C; et al. Novel Zinc Porphyrin*

Sensitizers for Dye-Sensitized Solar Cells: Synthesis and Spectral, Electrochemical, and Photovoltaic Properties. Chem. Eur. J. 2009, 15, 1403 – 1412. © 2009 John Wiley and Sons.

In DSSC, these porphyrin based compounds rely on $\pi \rightarrow \pi^*$ transitions to achieve electron transfer (diagram of which is shown in Figure 6). A porphyrin is modified with an electron donor and electron acceptor substituents. The compound is again coupled with an electrolyte, typically Co^{2+}/Co^{3+} complexes (see Figure 6), and placed between two electrodes, also TiO_2 and gold, to make the cell.[37, 38] The excitation in porphyrins arises from $\pi \rightarrow \pi^*$ transitions. As in the case of the ruthenium dyes, the excited porphyrin can either relax back to its ground state or inject an electron into the cathode surface. If an electron is injected, the porhyrin becomes oxidized. The porphyrin is then reduced by the electron donor substituent (nitrogen atom in the provided example). After the injected electron travels through the cell, it exits the anode and reduces Co^{3+} to Co^{2+}. The Co^{2+} then reduces the electron donor substituent of the porphyrin (nitrogen) to return the species to its original oxidation state. These porphyrin compounds can be assembled in in the cell in different ways, such as liquid crystals[39, 40] or as polymers[39, 41].



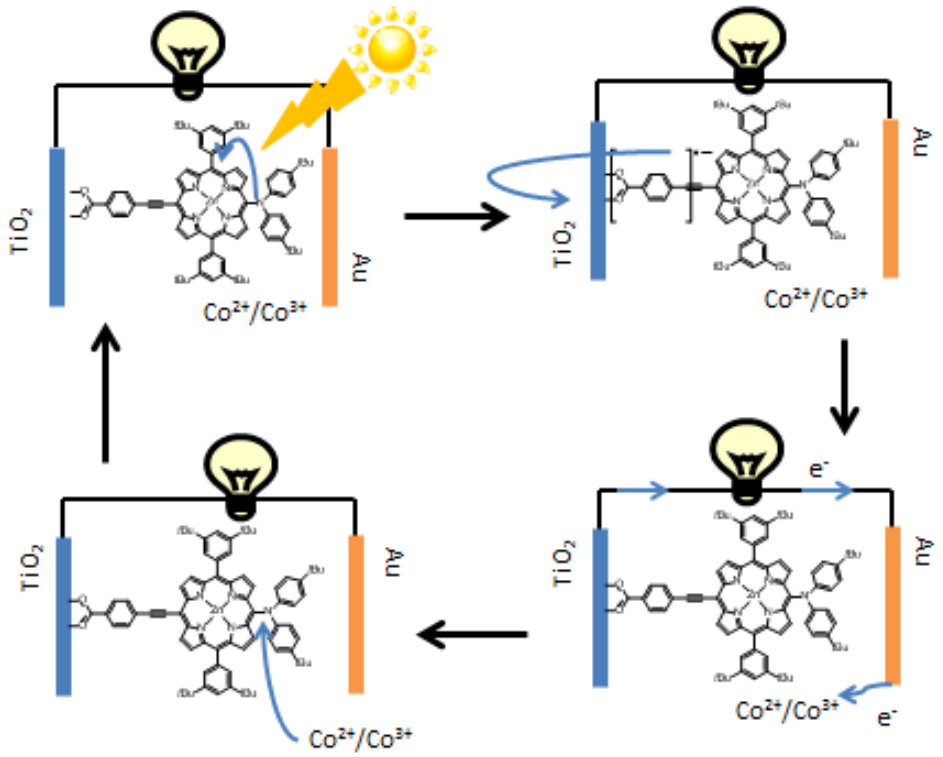


Figure 6. Top: Co(II) tris(bipyridene) complex used as the electrolyte in porphyrin based DSSC. Bottom: Typical dye sensitized solar cell based on porphyrin dyes shown with electron flow.

However, there are some points against the use of generic porphyrins in DSSC's mainly due to the absorbance spectrum. Like the ruthenium based dyes, porphyrins also experience absorbance decay after about 700 nm. Also there are large areas where porphyrins do not absorb at all (shown in Figure 5 spectrum between 500 and 600 nm). Since ruthenium and porphyrin dyes rely on two different types of electronic excitation, a possible remedy to improve absorbance over as much of the solar spectrum as possible (Figure 7) is to develop a compound that potentially contains both charge transfer, as in ruthenium dyes, and $\pi \rightarrow \pi^*$ electronic transitions, as in porphyrin dyes[42], which is the focus of this research.

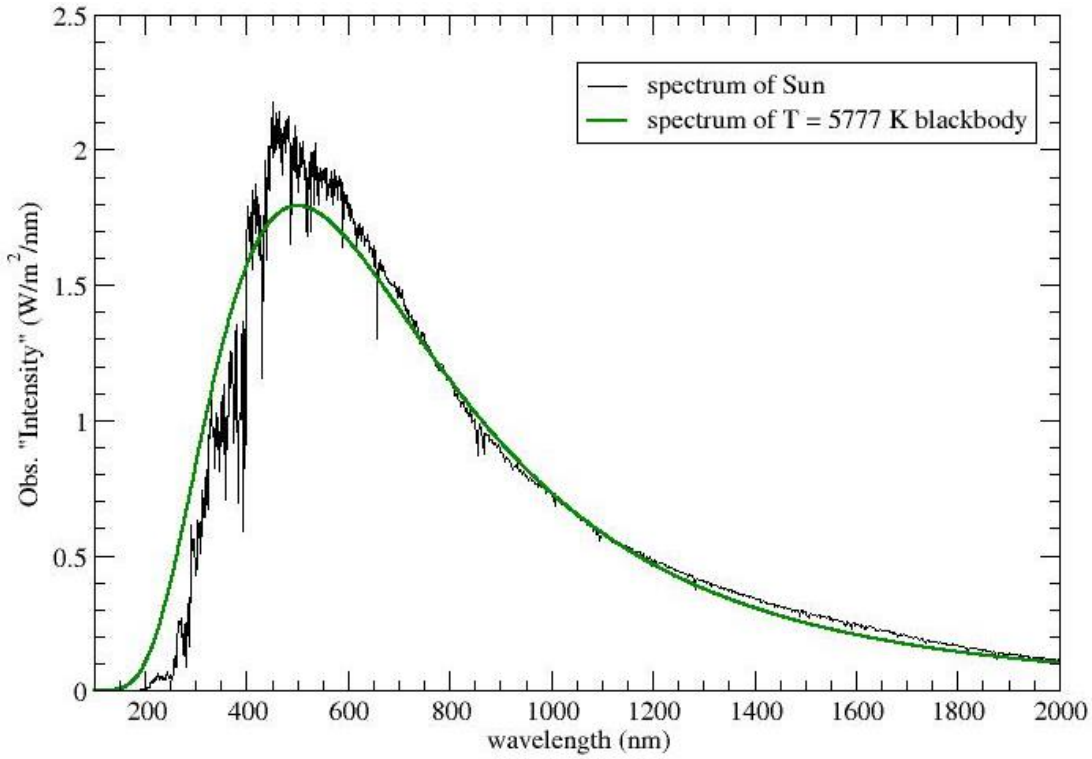


Figure 7. Solar emission spectrum (in black) and equivalent black-body radiation emission spectrum (in green)[43].

Methods:

In this project, we studied two ferrocenyl substituted tetraazaporphyrins, tetraferrocenyltetraazaporphyrin, ($TAP^{Fc}Mg$) and tetracyano-tetraferrocenyltetraazaporphyrin ($TAP^{FcCN}Mg$), as shown in Figure 8. The introduction of the organometallic ferrocenyl groups results in the possibility of charge transfer electronic transitions from the ferrocene d-orbitals to the π* orbitals of the tetraazaporphyrin[44].

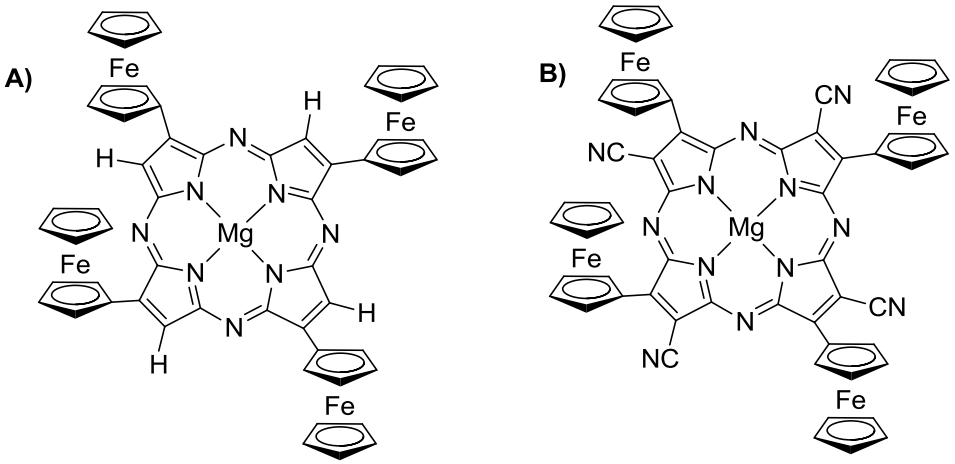


Figure 8a and 8b. The two compounds to be discussed in this study are shown. A: 2(3),7(8),12(13),17(18)-tetraferrocenyl-5,10,15,20-tetraazaporphyrinatomagnesium (TAP^{Fc}Mg). B: 2,7,12,17-tetracyano-3,8,13,18-tetraferrocenyl-5,10,15,20-tetraazaporphyrinatomagnesium (TAP^{FcCN}Mg).

There is some ambiguity with regards to the geometry of the compounds themselves, especially in TAP^{Fc}Mg since it is unknown which of the β positions the ferrocene substituent will substitute, due to the potential to form multiple positional

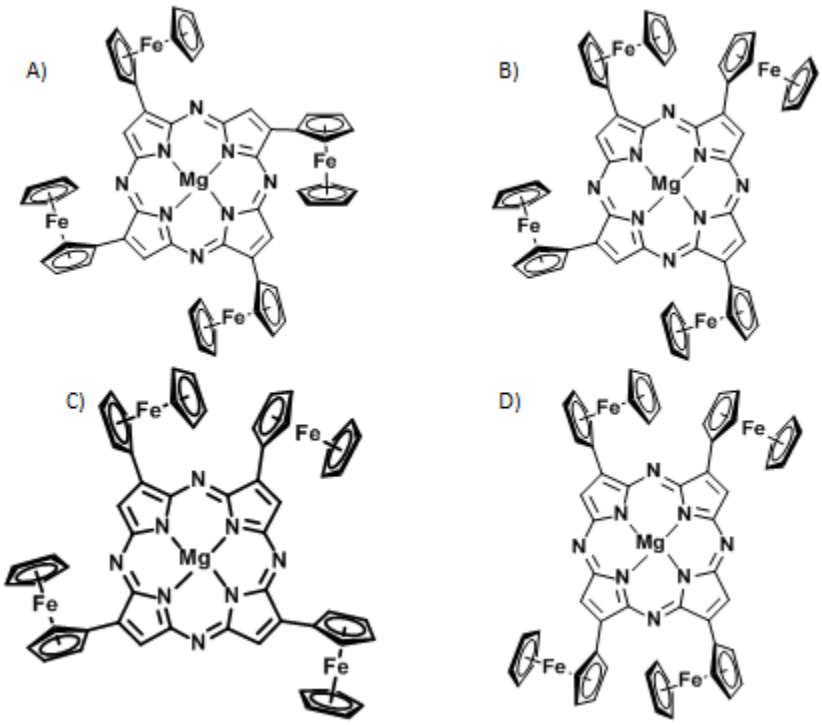


Figure 9a. The four possible positional isomers of TAP^{Fc}Mg: A) 3,8,13,18-tetraferrocenyl-5,10,15,20-tetraazaporphyrinatomagnesium; B) 2,8,13,18-tetraferrocenyl-5,10,15,20-tetraazaporphyrinatomagnesium; C) 2,7,13,18-tetraferrocenyl-5,10,15,20-tetraazaporphyrinatomagnesium; D) 2,8,12,18-tetraferrocenyl-5,10,15,20-tetraazaporphyrinatomagnesium.

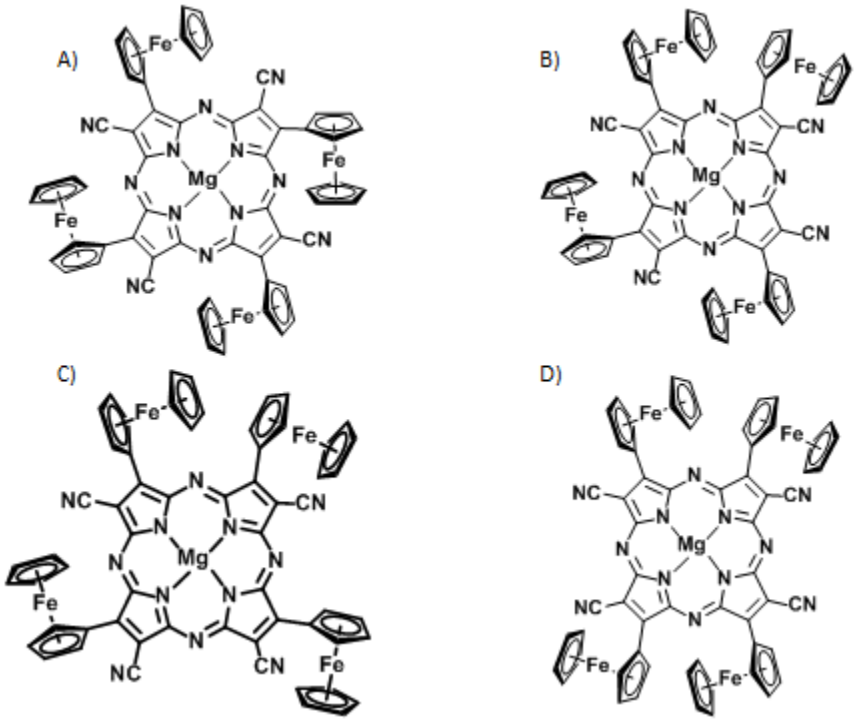


Figure 9b. The four possible positional isomers of TAP^{FcCN}Mg. A) 2,7,12,17-tetracyano-3,8,13,18-tetraferrocenyl-5,10,15,20- tetraazaporphyrinatomagnesium; B) 2,8,12,17-tetracyano-3,7,13,18-tetraferrocenyl-5,10,15,20- tetraazaporphyrinatomagnesium; C) 2,8,13,17-tetracyano-3,7,12,18-tetraferrocenyl-5,10,15,20-tetraazaporphyrinatomagnesium; D) 2,8,12,18-tetracyano-3,7,13,17-tetraferrocenyl-5,10,15,20- tetraazaporphyrinatomagnesium.

isomers. There are four possible positional isomers that result in varying positions of the ferrocene and cyano (or hydrogen) groups around the tetraazaporphyrin ring. This would lead one to assume that all four isomers needed to be discussed (see Figure 9). While the problem of identifying isomers of similar compounds has been investigated[45], experimentally we see something simpler. When in a mixture, isomers A and D of the cyano sybstituted compound separate into a non-polar fraction and isomers B and C of

the cyano substituted compound separate into a polar fraction. However, this can only be done for the cyano substituted compound ($TAP^{FcCN}Mg$), since the hydrogen substituted compound, $TAP^{Fc}Mg$ is not polar enough to allow for this type of separation. This property allows the isomers to be separated, at least partially, from

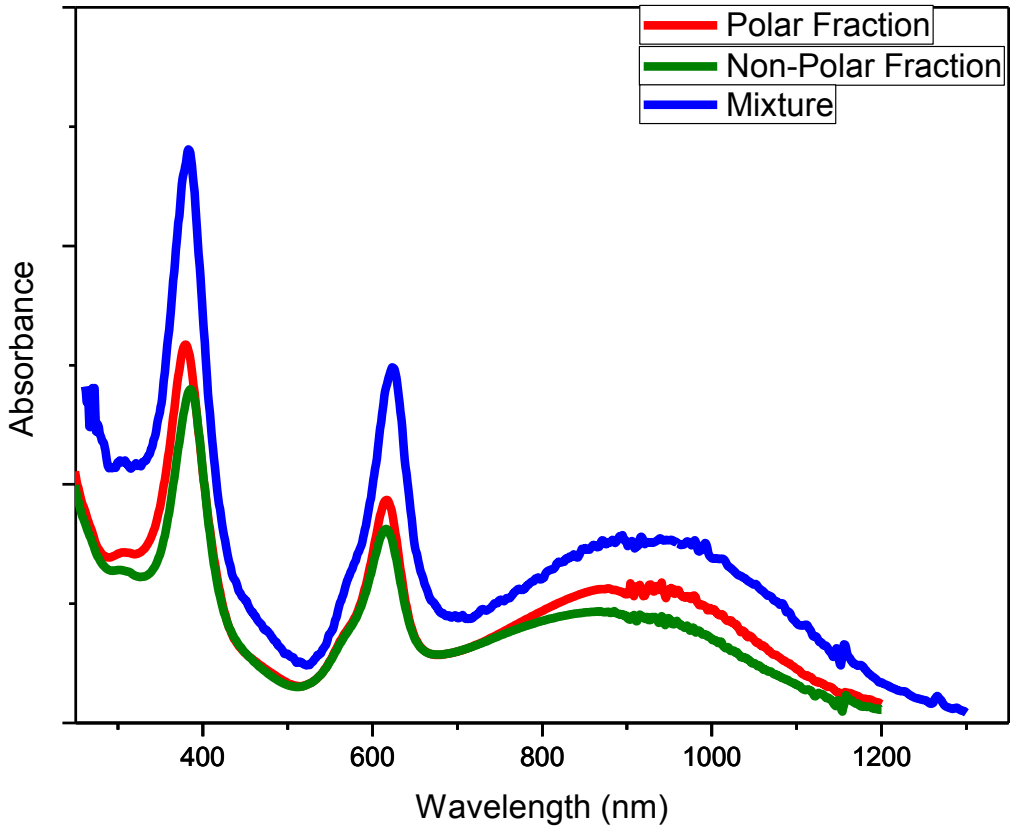


Figure 10. UV-Vis spectra for $TAP^{FcCN}Mg$ and separated isomers. Blue line: non-separated compound, Red line: Polar fraction, Green line: non-polar fraction. Taken from the research lab of Dr. Viktor Nemykin by Anatolii Pucharel and Tony Wertish.

one another after synthesis. Since, these two fractions have very similar absorption properties, it is assumed that the spectroscopic results of one isomer will be similar to another isomer, and give an acceptable picture of the compound as a whole (Figure 10).

To make the calculations less computationally intensive, the highest symmetry isomer of each compound was selected for calculations. This is the isomer that contains alternating hydrogen/cyanide and ferrocene substituents (isomer A: 3,8,13,18-tetraferrocenyl-5,10,15,20-tetraazaporphyrinatomagnesium and 2,7,12,17-tetracyano-3,8,13,18-tetraferrocenyl-5,10,15,20- tetraazaporphyrinatomagnesium). The choice of exchange-correlation functional used for the calculations, however, could not immediately be decided since the compounds in question potentially contained both charge transfer and $\pi \rightarrow \pi^*$ electronic transitions. When using a pure correlation functional, the calculated transition energies of charge transfer transitions are typically underestimated (lower energy, higher wavelength) [46]. In order to achieve a better agreement between theoretical and experimental data, some percentage of Hartree-Fock (HF) exchange is introduced into an exchange-correlation functional to make a hybrid in the exchange-correlation functional. However, the introduction of too high a percentage of HF exchange into the exchange-correlation functional will result in all transition energies to be overestimated (high energy, low wavelength) [47]. Because of this dilemma, a hybrid functional needs to be selected that has the correct balance of the exchange part and correlation part of the functional to achieve an acceptable compromise to the disagreement of calculated transition energies. By convention, acceptable results between theory and experiment occur when the difference between theoretical and experimental results is less than 0.1 eV, or about 800 cm^{-1}. In this study four different exchange-correlational functionals were tested: i) Becke's exchange functional with Perdew and Wang's gradient corrected correlation functional[48, 49] (BPW91: 0% HF); ii) Becke's exchange functional with Perdew's correlation functional[48, 50] (BP86: 0% HF);

iii) Becke's three parameter exchange functional with Lee, Yang, and Parr's correlation functional[51, 52] (B3LYP: ~20% HF); iv) and Burke, Perdew, and Ernzerhof's functional with their gradient corrected correlation functional[53] (PBE1PBE or PBE0: ~25% HF). Two pure DFT functionals were used to confirm that any visible error was due to lack of HF exchange, rather than correlation, used in the calculation. Geometry optimization (computation time: 1-2 weeks with 8 CPUs) and time-dependent density functional theory (TDDFT) calculations (computation time: 2-4 days with 8 CPUs and 100 states calculated) were run using all four functionals.

The basis set used for all calculations was the LANL2DZ basis set. This was chosen due to the fact that the compounds that were studied are very large and using a large basis set would be essentially impossible, even on a supercomputer. The LANL2DZ set utilized effective core potentials for second row and above elements, thus removing core electrons form the calculation and reducing the number of primitive gaussians to be calculated (first row elements are calculated with the Dunning/Huzinaga valence double-zeta, D95V, basis set). Even with the LANL2DZ basis set, 1980 and 2164 primitive gaussians need to be considered for calculation for $TAP^{Fc}Mg$ and $TAP^{FcCN}Mg$, respectively. All calculations were run both in gas phase and in dichloromethane (DCM). The calculations done in DCM were conducted using a self-consistent reaction field method, specifically, Tomasi's Polarized Continuum Model (PCM), where the compound sits in a cavity made up of interlocking spheres in a uniform dielectric constant[54, 55]. The polarization effect of the solvent on the compound is then calculated by numerical integration. Since the compound in a solution is a "real world"

model, it is the DCM calculations that will be compared to experimental data. Once an acceptable agreement was found between the PCM-TDDFT calculation of a particular functional and experimental data, single point energy calculations were run (computation time: 12-24 hours with 8 CPUs) using that particular functional to determine the electronic structure of the compound and make band assignments of the PCM-TDDFT calculations and identify possible charge transfer and $\pi \rightarrow \pi^*$ electronic transitions. All calculations were calculated with the Gaussian 09 software package[56]; all data was plotted with OriginLab software[57] with data taken from Gaussian 09 and spectra generated from GaussView v5[58] (With a band width of 0.1 eV for all TDDFT and PCM-TDDFT data); molecular orbitals were analyzed with the QMForge application while their contours were generated with the GaussView v5 molecular viewer[58].

Results:

The final goal of the study was to identify and characterize the electronic transitions of the two tetraazaporphyrin compounds being discussed. The idea was to design compounds that would contain both charge transfer and $\pi \rightarrow \pi^*$ electronic transitions, thus potentially maximizing solar spectrum absorption (sample transitions shown in Figure 11). In a charge transfer transition the orbital location of the ground state is centered around an atom or groups of atoms that are different from the excited state (a common example include metal-to-ligand charge transfer, where an electron in a metal centered orbital is excited to a ligand centered orbital). A $\pi \rightarrow \pi^*$ electronic transition occurs when an electron is excited from a bonding to antibonding orbital of a π system.

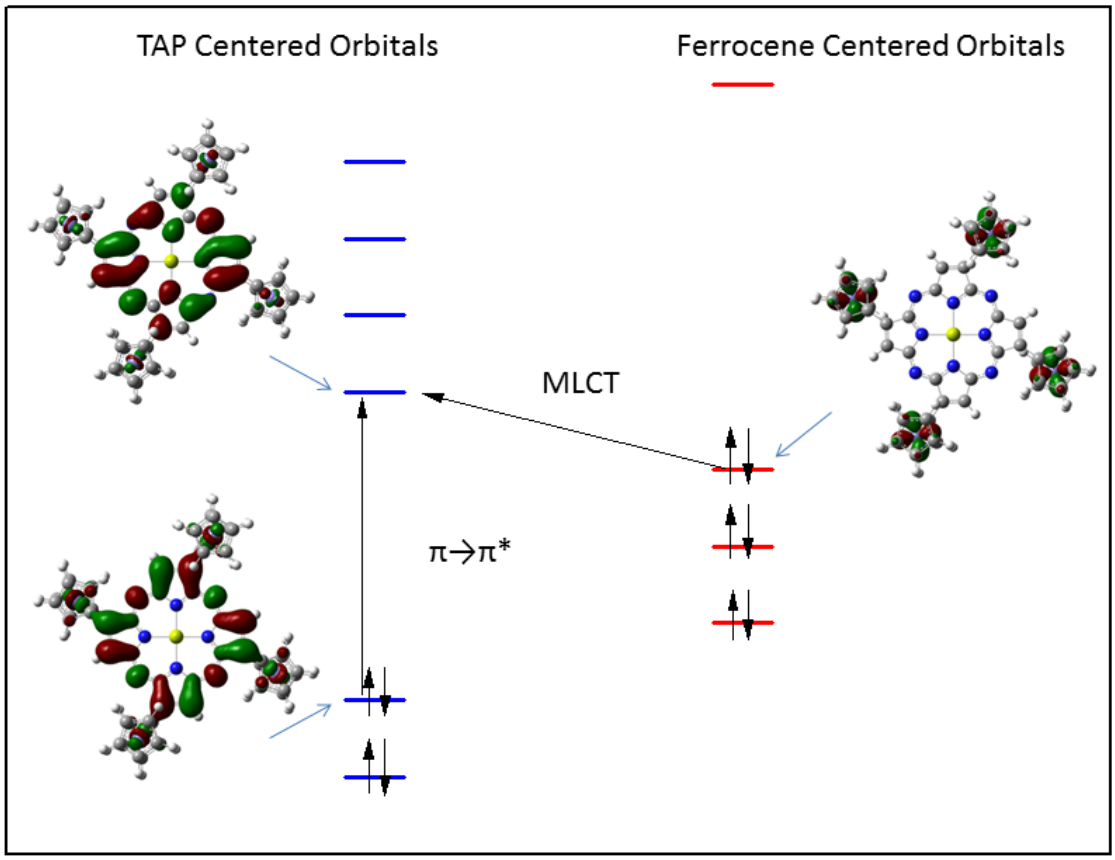


Figure 11. Generic energy diagram of the frontier orbitals of TAP^{Fc}Mg is shown. Each line represents a molecular orbital and has been separated by type for clarity. In this example, π orbitals are indicated in blue (for this study, these would correspond to tetrazaporphyrin centered orbitals; sample π orbital shown to left), and the substituent orbitals are in red (for this study, these would correspond to ferrocene centered orbitals; sample ferrocene orbital shown to right). A π⟶π transition would be indicated, as shown, by a transfer from blue to blue (tetraazaporphyrin to tetraazaporphyrin) and a charge transfer transition would be indicated by a red to blue (ferrocene to tetraazaporphyrin). A blue to red (tetraazaporphyrin to ferrocene) transition would also count as a charge transfer transition, but did not appear as part of the major transitions that were calculated.*

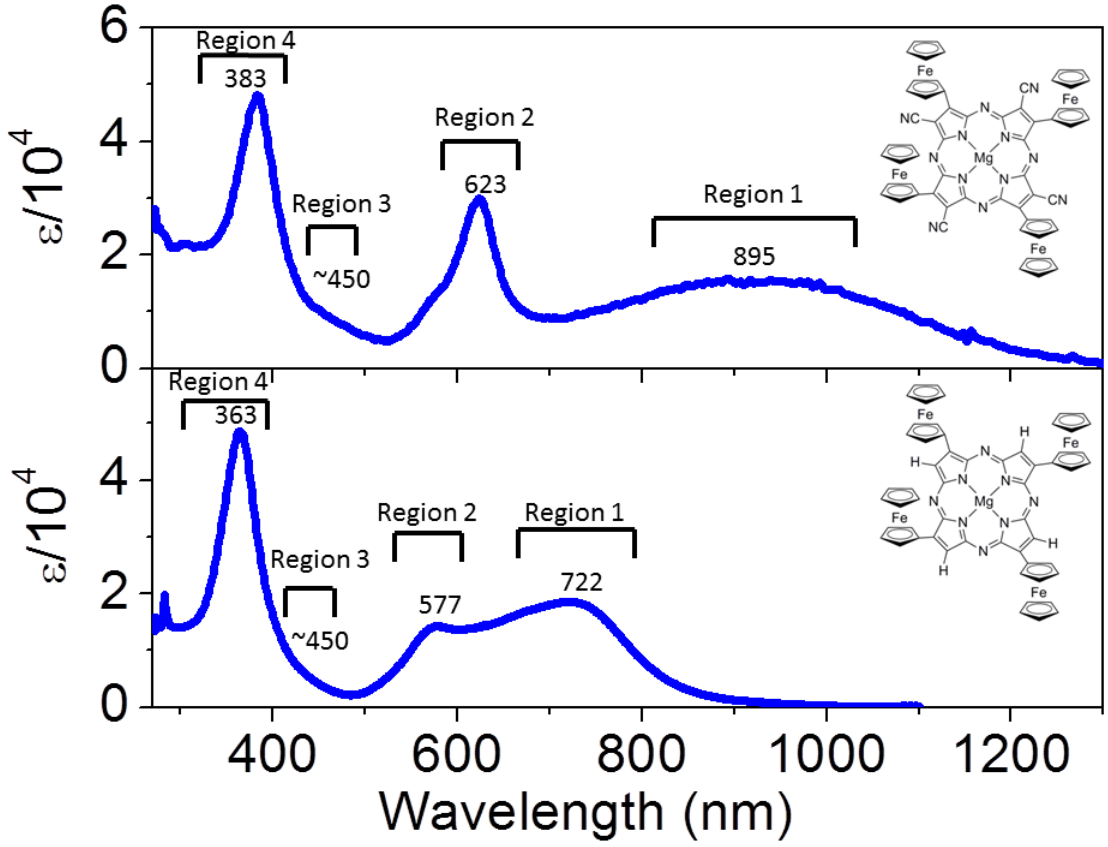
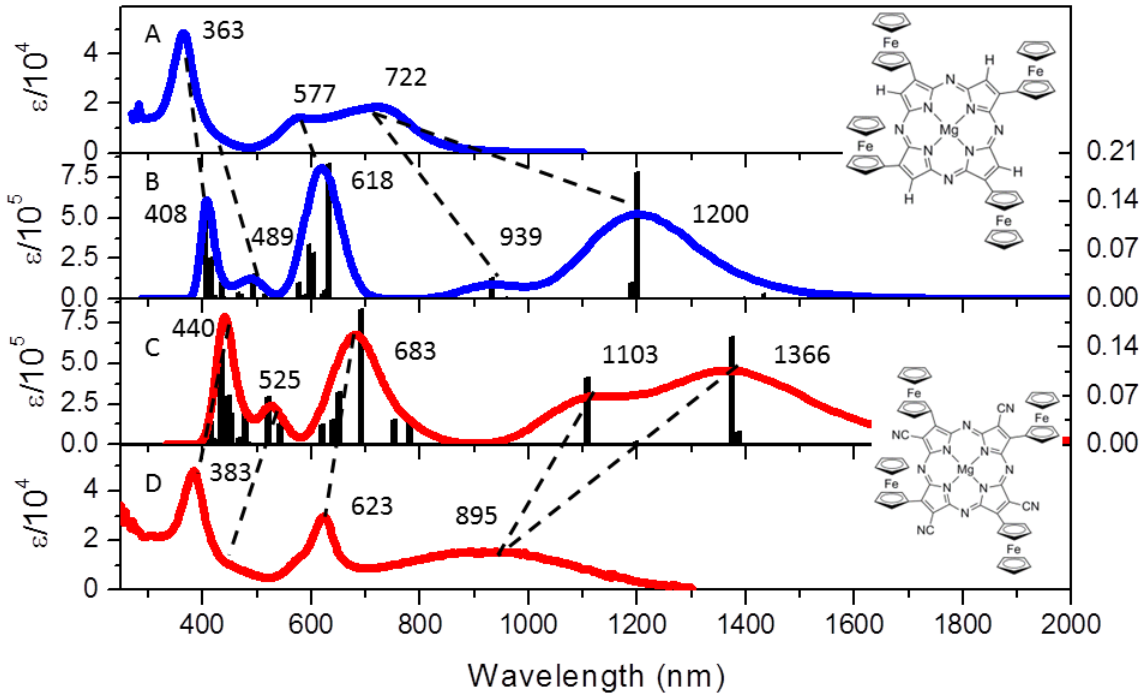


Figure 12. Experimentally obtained UV-Vis-NIR spectrum of the two compounds in question is shown, with TAP^{FcCN}Mg shown at top and TAP^{Fc}Mg shown at bottom. Major absorbance peaks are labeled and separated by region.

The experimental absorption spectra (Figure 12) of the two tetraazaporphyrins each contain four regions of interest. First, the TAP^{Fc}Mg UV-Vis-NIR spectrum contains broad peak centered at 722 nm (13850 cm^{-1}; Region 1), a less defined peak at 577 nm (17331 cm^{-1}; Region 2), and a sharp, intense peak at 363 nm (27548 cm^{-1}; Region 4). Second, the TAP^{FcCN}Mg UV-Vis-NIR spectrum contains a very broad peak, much broader than in the TAP^{Fc}Mg spectrum, centered at 895 nm (11173 cm^{-1}; Region 1), a sharp peak at 623 nm (16051 cm^{-1}; Region 2), and a sharp and intense peak at 383 nm (26109 cm^{-1}; Region 4). Region 3 consists of low intensity shoulders, centered

approximately around the 450 nm region (22222 cm^{-1}), that are most likely covered by the intense region 4 peaks. Region 3 does not clearly appear in the experimental spectrum, but does appear in the PCM-TDDFT calculations. For each compound, these four regions, along with their relative profiles were compared to computationally generated spectra using the four previously mentioned functionals.



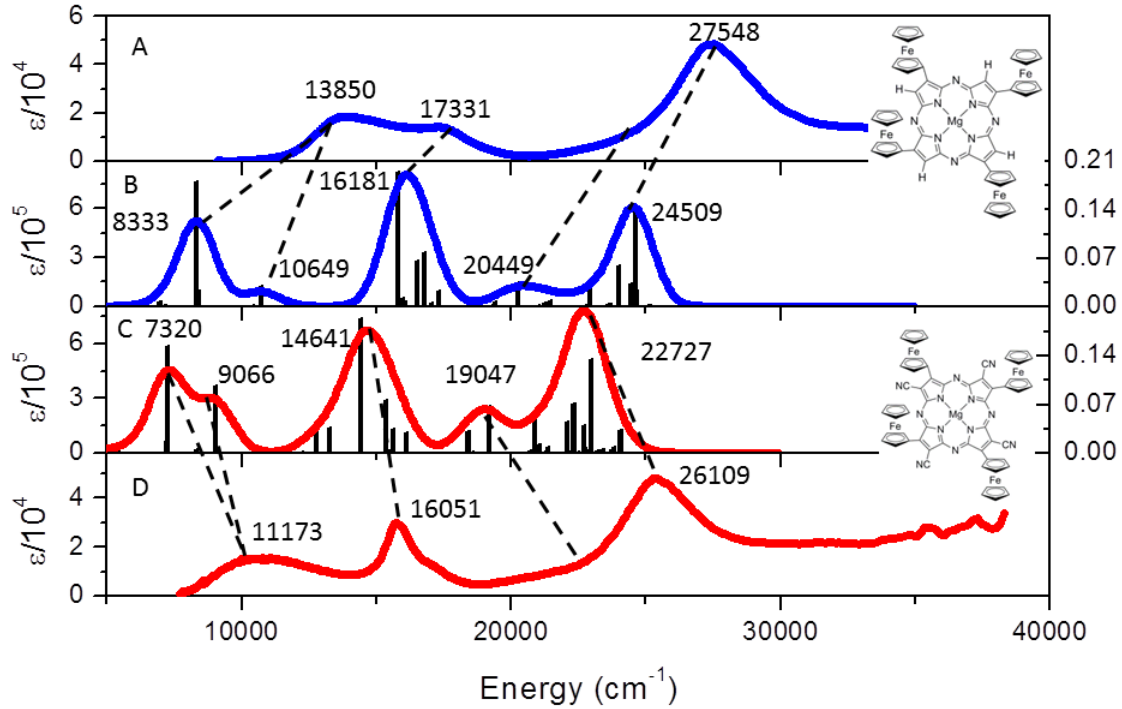
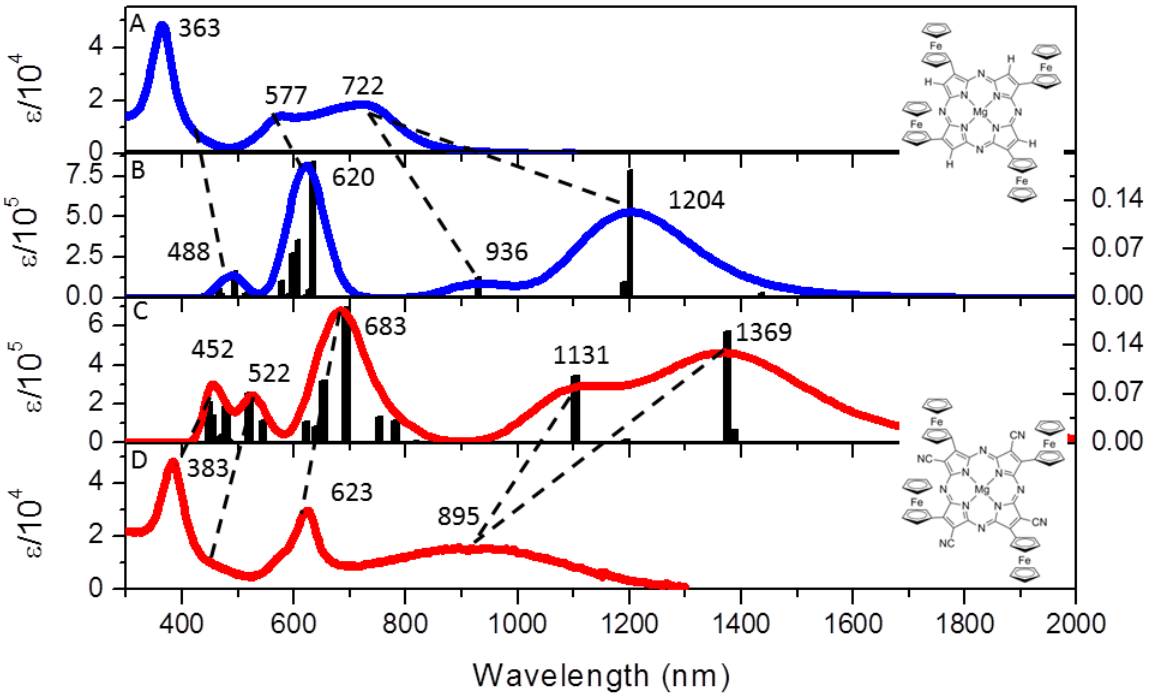


Figure 13a (spectrum in nm) and 13b (spectrum converted to energy (cm^{-1})). Experimental vs. theoretical data for BPW91 exchange-correlation functional. A: $TAP^{Fc}Mg$ experiment; B: $TAP^{Fc}Mg$ PCM-TDDFT; C: $TAP^{FcCN}Mg$ PCM-TDDFT; D: $TAP^{FcCN}Mg$ experiment. Black dashed lines sown to match experimental peaks to theoretical peaks.

The results of the theoretical PCM-TDDFT calculations using the BPW91 exchange-correlation functional are presented in Figure 13 (these results were previously calculated using 150 excited states for TDDFT and PCM-TDDFT calculations). The $TAP^{Fc}Mg$ calculation gave a sharp peak at 408 nm (24508 cm^{-1}), a small peak at 489 nm (20449 cm^{-1}), another sharp peak at 618 nm (16181 cm^{-1}), a small, relatively broad peak at 939 nm (10649 cm^{-1}), and an intense broad peak at 1200 nm (8333 cm^{-1}). From experiment to calculation, region 1 splits from one defined absorbance peak into two defined absorbance peaks and shifts from 13850 to 10649 and 8333 cm^{-1}, region 2 shifts from 17331 to 16181 cm^{-1}, region 3 becomes visible but relatively weak at 20449 cm^{-1},

and region 4 shifts from 27548 to 24509 cm^{-1}. The $TAP^{FcCN}Mg$ calculation gave a sharp peak at 440 nm (22727 cm^{-1}), a small peak at 525 nm (19047 cm^{-1}), a second sharp peak at 683 nm (14641 cm^{-1}), a shoulder at about 1103 nm (9066 cm^{-1}), and a broad, intense peak at 1366 nm (7320 cm^{-1}). From experiment to calculation, region 1 also splits from one to two defined absorbance peaks and shifts from 11173 to 7230 and 9066 cm^{-1}, region 2 shifts from 16051 to 14641 cm^{-1}, region 3 becomes visible and relatively intense at 19047 cm^{-1}, and region 4 shifts from 26109 to 22727 nm. The largest difference in theoretical and experimental peak locations being is over 5000 cm^{-1}, which is well outside our limit of ~800 cm^{-1} for acceptable data. Also, considering the peak splitting that occurs in Region 1 between theoretical and experimental spectrum, it can be concluded that the BPW91 functional gives poor agreement for these two compounds.



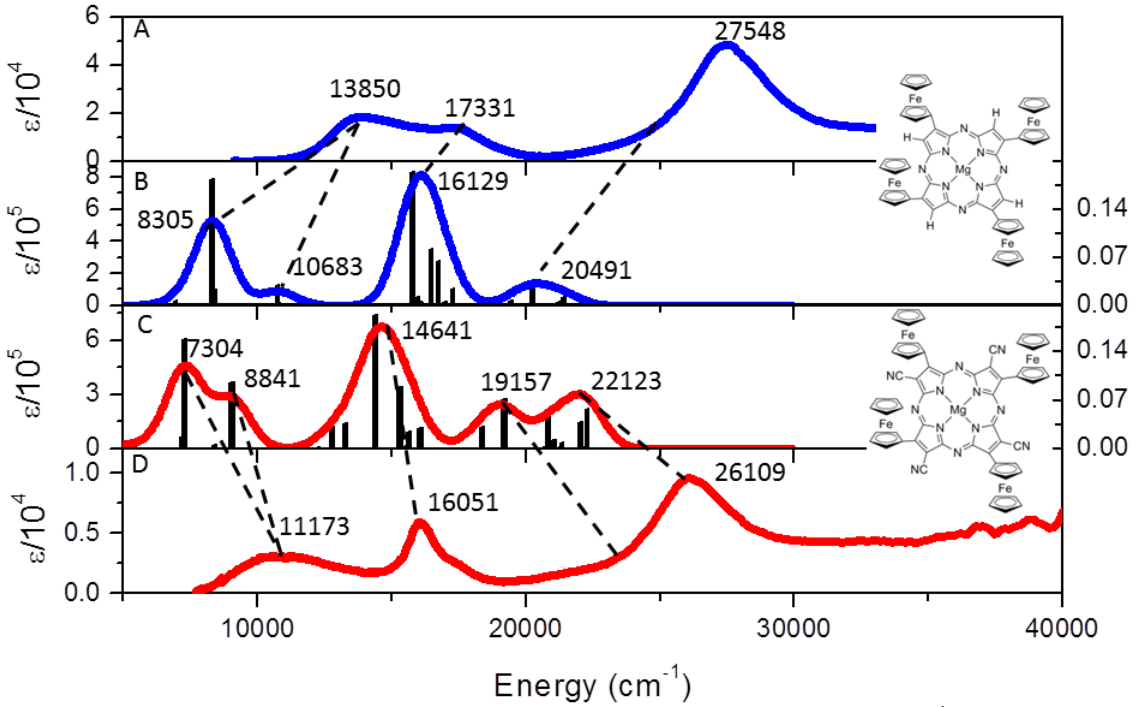


Figure 14a (spectrum in nm) and 14b (spectrum converted to energy (cm^{-1})). Experimental vs. theoretical data for BP86 exchange-correlation functional. A: $TAP^{Fc}Mg$ experiment; B: $TAP^{Fc}Mg$ PCM-TDDFT; C: $TAP^{FcCN}Mg$ PCM-TDDFT; D: $TAP^{FcCN}Mg$ experiment. Black dashed lines sown to match experimental peaks to theoretical peaks.

To prove the poor agreement originated from the lack of Hartree-Fock exchange in the exchange-correlation functional, a second pure exchange-correlation functional was used. For BP86 exchange-correlation functional, presented in Figure 14, the calculations for $TAP^{Fc}Mg$ gave a small peak at 488 nm (20491 cm^{-1}), a sharp peak at 620 nm (16129 cm^{-1}), a small peak at 936 nm (10683 cm^{-1}), and a broad, relatively intense, peak at 1204 nm (8305 cm^{-1}). From experiment to calculation, region 1 again splits into two defined peaks, shifting from 13850 to 8305 and 10683 cm^{-1}, region 2 shifts from 17331 to 16129 cm^{-1}, region 3 becomes visible at 20491 cm^{-1}, and region 4 does not actually appear in the theoretical spectrum because a small number of excited states were considered in the BP86 calculations (100 Excited states compared to BPW91 150 excited

states). The calculations for the $TAP^{FcCN}Mg$ gave two small peaks at 452 and 522 nm (22123 and 19157 cm^{-1}, respectively), a sharp peak 683 nm (14641 cm^{-1}), an intense shoulder at 1131 nm (8841 cm^{-1}), and a very intense broad peak at 1369 nm (7304 cm^{-1}). From experiment to calculation, region 1 again splits into two defined peaks and shifts from 11173 to 7304 and 8841 cm^{-1}. Region 2 becomes broader and shifts from 16051 to 14641 cm^{-1}, region 3 becomes visible at 19157 cm^{-1}, and region 4 appears much weaker in intensity than it does in the experimental spectrum and shifts from 26109 to 22123 cm^{-1}. Even though 100 excited states were calculated as part of the initial PCM-TDDFT calculation, the missing region 4 peak in the $TAP^{Fc}Mg$ calculation could mean that more excited states need to be calculated to accurately calculate this peak. Also, the region 4 peak in the $TAP^{FcCN}Mg$ calculation is calculated to be much less intense than in the experiment. Again, this could most likely mean the PCM-TDDFT calculation needs more excited states to be calculated. The largest difference between theoretical and experimental peak locations is again over 5000 cm^{-1}, indicating very poor agreement between theory and experiment using the BP86 functional. Also, there is again peak splitting of the Region 1 peak between theory and experiment, also indicating poor agreement. These previous two results show some reasonable agreement between the higher energy transitions (< 600 nm transitions) and very poor agreement between lower energy transitions (> 800 nm transitions). This specific combination of acceptable and poor agreement indicates that the lower energy transitions are predominately charge transfer transitions and that the higher energy transitions are predominately $\pi \rightarrow \pi^*$ transitions, based on the previous statement that lack of HF exchange will underestimate charge transfer transition energies.

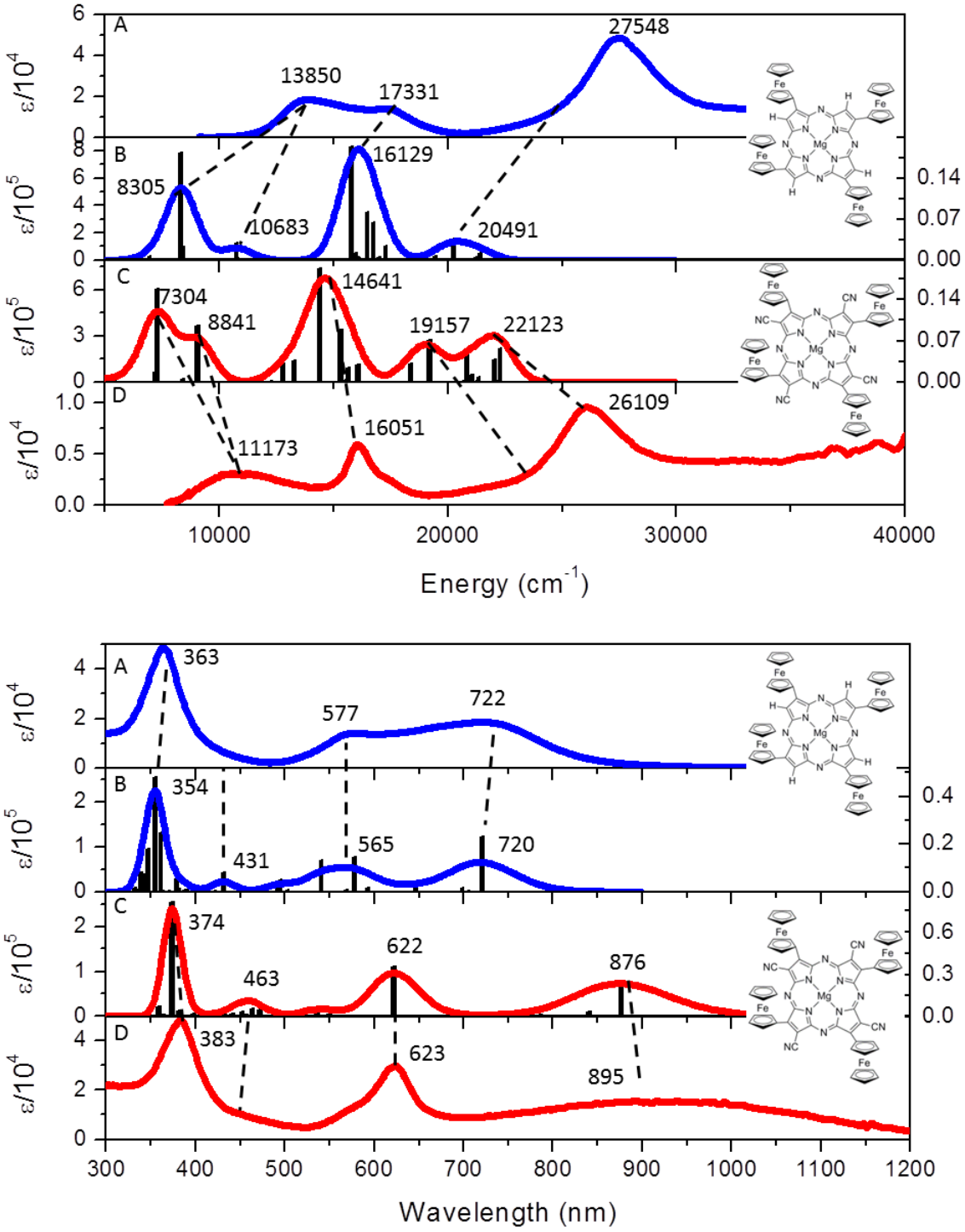


Figure 15a (spectrum in nm) and 15b (spectrum converted to energy (cm^{-1})). Experimental vs. theoretical data for B3LYP exchange-correlation functional. A: $TAP^{Fc}Mg$ experiment; B: $TAP^{Fc}Mg$ PCM-TDDFT; C: $TAP^{FcCN}Mg$ PCM-TDDFT; D:

TAP^{FcCN}Mg experiment. Black dashed lines sown to match experimental peaks to theoretical peaks.

The B3LYP (~20% HF) calculations that are presented in Figure 15 resulted in the best agreement between theory and experiment. The TAP^{Fc}Mg calculation gave a sharp peak at 354 nm (28248 cm^{-1}), a small peak at 431 nm (23201 cm^{-1}), a relatively broad peak at 565 nm (17699 cm^{-1}), and a second relatively broad peak at 720 nm (13888 cm^{-1}). From experiment to calculation, region 1 shifted from 13850 to 13888 cm^{-1}, region 2 shifts from 17331 to 17699 cm^{-1}, region 3 becomes visible, although still relatively weak at 23201 cm^{-1}, and region 4 shifts from 27548 to 28248 cm^{-1}. The TAP^{FcCN}Mg calculation gave a sharp peak at 374 nm (26737 cm^{-1}), a small peak at 463 nm (21598 cm^{-1}), a relatively sharp peak at 622 nm (16077 cm^{-1}), and a relatively broad peak at 876 nm (11415 cm^{-1}). From experiment to calculation, region 1 shifts from 11173 to 11415 cm^{-1}, region 2 shifts from 16051 to 16077 cm^{-1}, region 3 become visible, and still relatively weak at 21598 cm^{-1}, and region 4 shifts from 26109 to 26737 cm^{-1}. The largest difference between the theoretical and experimental peak locations is between the calculated and experimental Region 1 peaks of TAP^{Fc}Mg, with a difference of 700 cm^{-1}, with the difference between the remaining peaks being significantly smaller. This shows that using the B3LYP functional provides excellent agreement between theory and experiment for these two compounds.

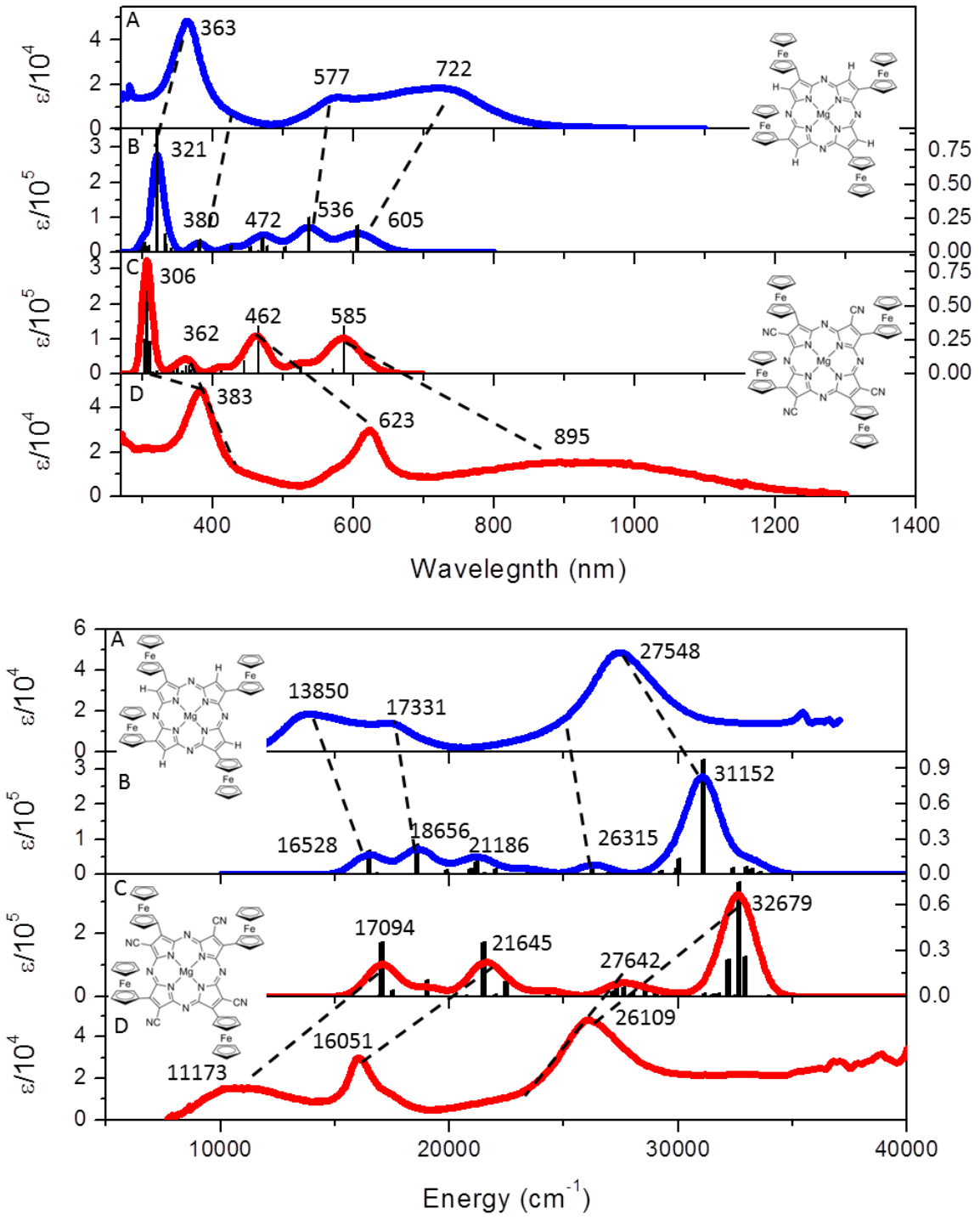


Figure 16a (spectrum in nm) and 16b (spectrum converted to energy (cm^{-1})). Experimental vs. theoretical data for PBE1PBE exchange-correlation functional. A: $TAP^{Fc}Mg$ experiment; B: $TAP^{Fc}Mg$ PCM-TDDFT; C: $TAP^{FcCN}Mg$ PCM-TDDFT; D: $TAP^{FcCN}Mg$ experiment. Black dashed lines sown to match experimental peaks to theoretical peaks.

The PBE1PBE (~25% HF), as expected, overestimated the transition energies (shown in Figure 16), resulting in lower wavelength peaks being reported. The $TAP^{Fc}Mg$ calculation gave a sharp peak at 321 nm (31152 cm^{-1}) and a series of four relatively small peaks at 380, 472, 536, and 605 nm (26315, 21186, 18656, and 16528 cm^{-1}, respectively). From experiment to calculation, region 1 shifts from 13850 to 16528 cm^{-1} and decreases in intensity, while becoming less broad. Region 2 shifts from 17331 to 18656 cm^{-1}. Region 3 becomes visible, while still weak, at 26315 cm^{-1}, and region 4 shifts from 27548 to 31152 cm^{-1}. The $TAP^{FcCN}Mg$ calculation gave a sharp peak at 306 nm (32679 cm^{-1}), a very small peak at 362 nm (27642 cm^{-1}), and two small peaks at 462 and 585 nm (21645 and 17094 cm^{-1}, respectively). From experiment to calculation, region 1 shifts from 11173 to 17094 cm^{-1}, region 2 shifts from 16051 to 21645 cm^{-1}, region 3 becomes visible, but weak at 27642 cm^{-1}, and region 4 shifts from 26109 to 32679 cm^{-1}. With the largest difference between theoretical and experimental peak locations being just under 6000 cm^{-1}, the PBE1PBE functional gives poor agreement for these compounds. With these transitions all being significantly overestimated, the testing of different hybrid functionals can stop, since testing with hybrid functionals having a greater Hartree-Fock exchange than PBE1PBE would only increase the calculated energies of the transitions.

With the B3LYP functional shown to have the best agreement between experimental and theoretical results, further calculations were done using the B3LYP functional to determine the orbitals involved in the aforementioned transitions (Figures 17 and 18), as well as their orbital composition, how much does each atom or group of atoms contribute to a particular molecular orbital (shown in Figure 19).

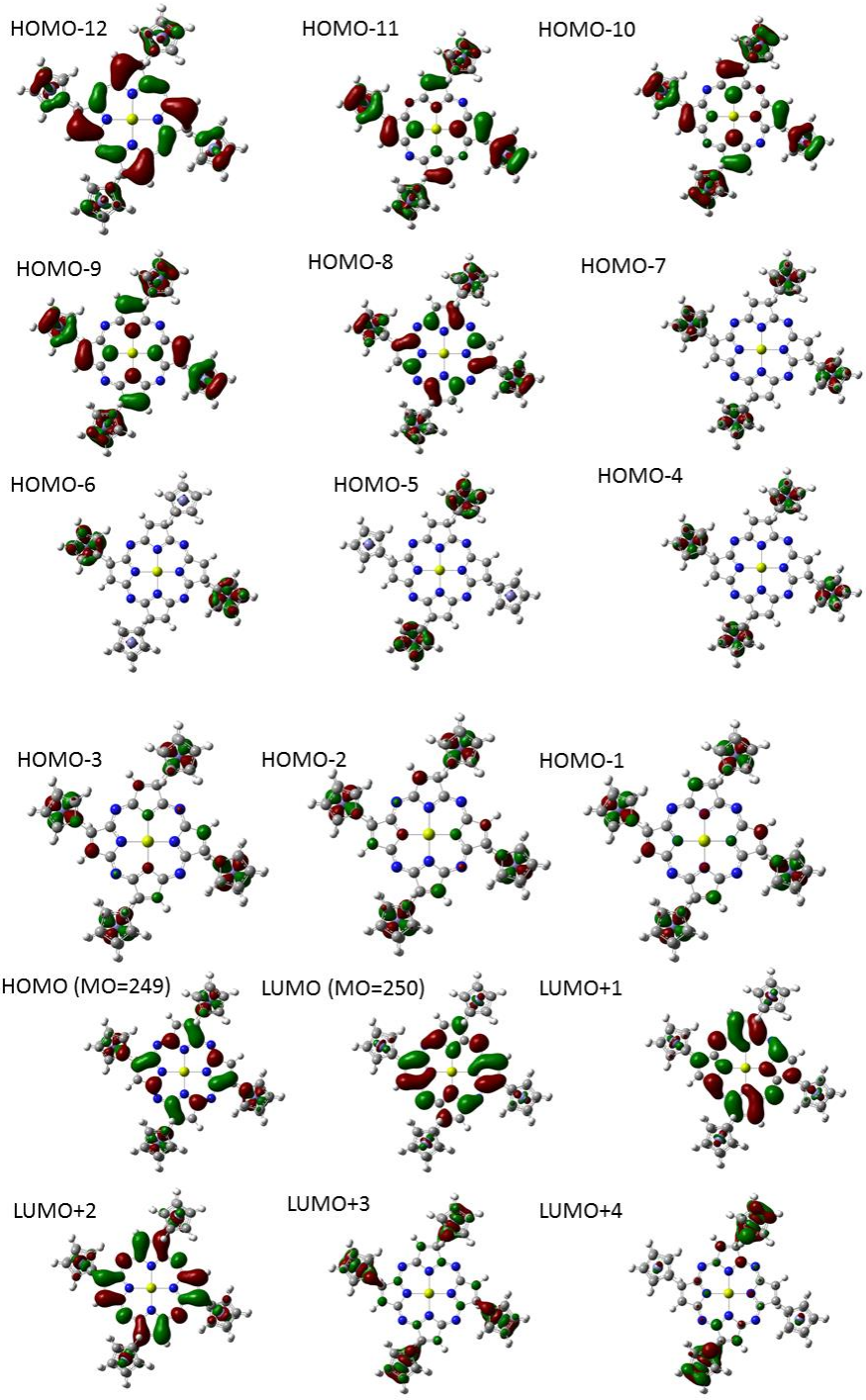


Figure 17. Frontier orbitals of TAP^{Fc}Mg are shown. Many of these orbitals are involved in the major electronic transitions that make up the absorbance spectrum.

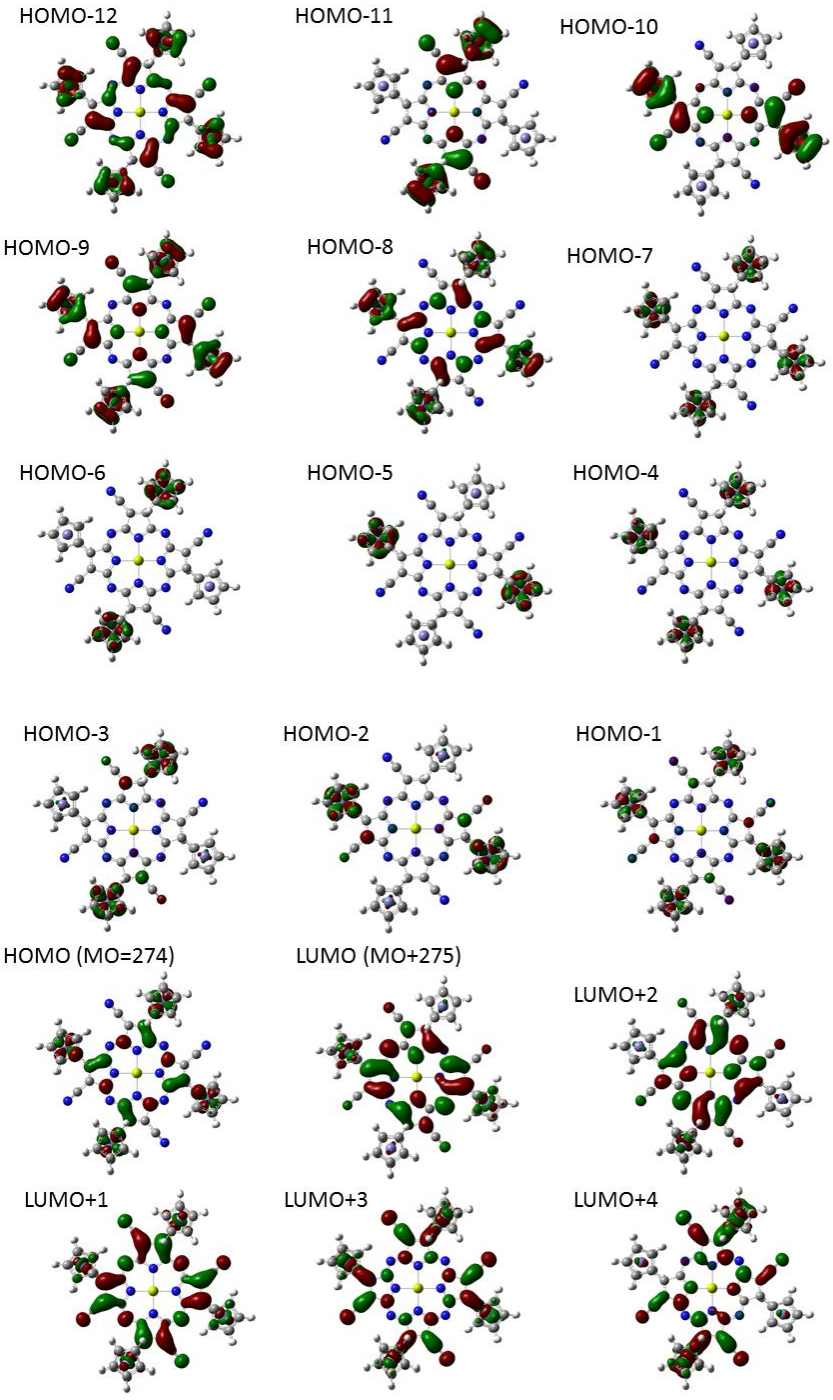
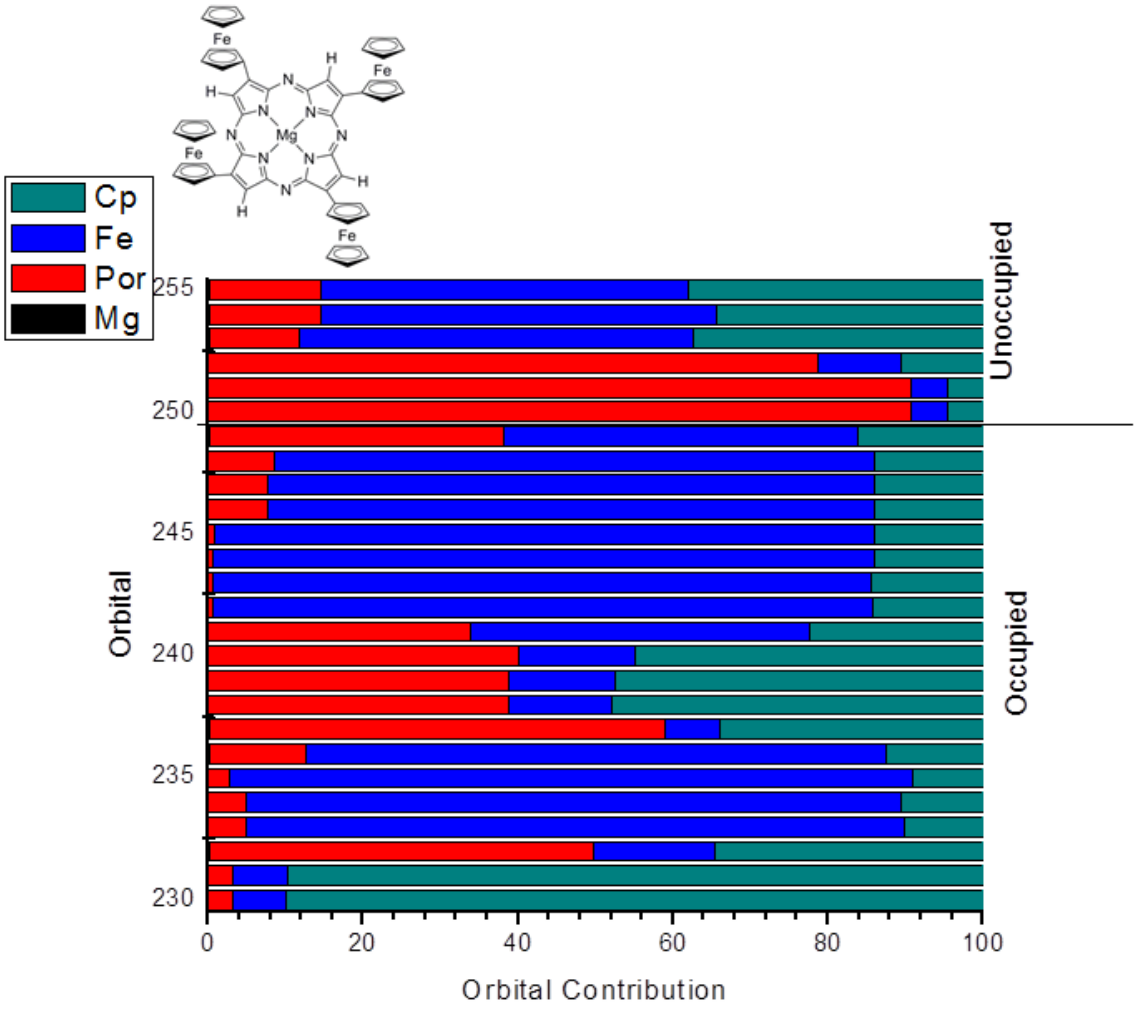


Figure 18. Frontier orbitals of TAP^{FcCN}Mg are shown. Many of these orbitals are involved in the electronic transitions that make up the absorbance spectrum.


Cp
Fe
Por
Mg
Fe
Fe
Fe
Fe
Mg
Unoccupied
Occupied
Orbital
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250
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240
235
230
0
20
40
60
80
100
Orbital Contribution

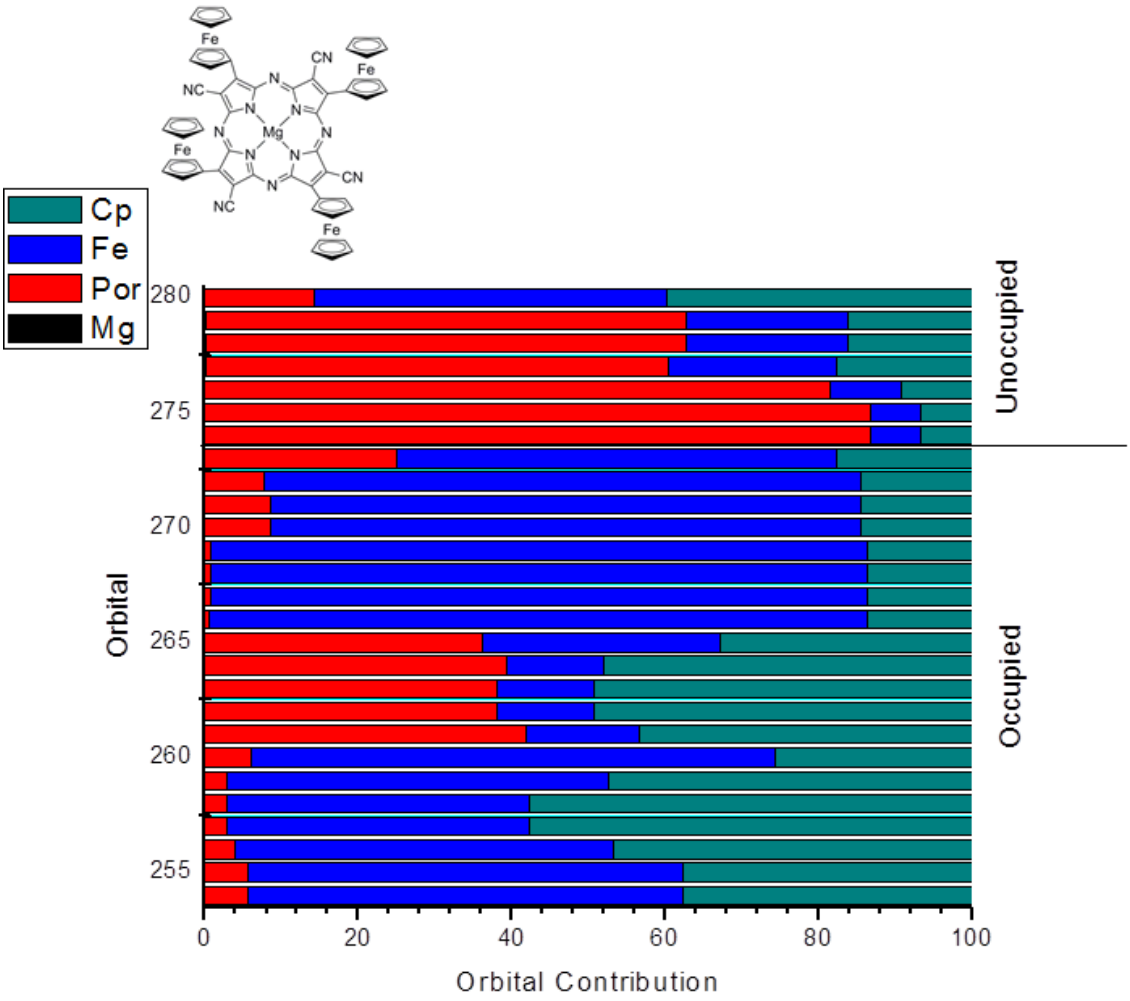
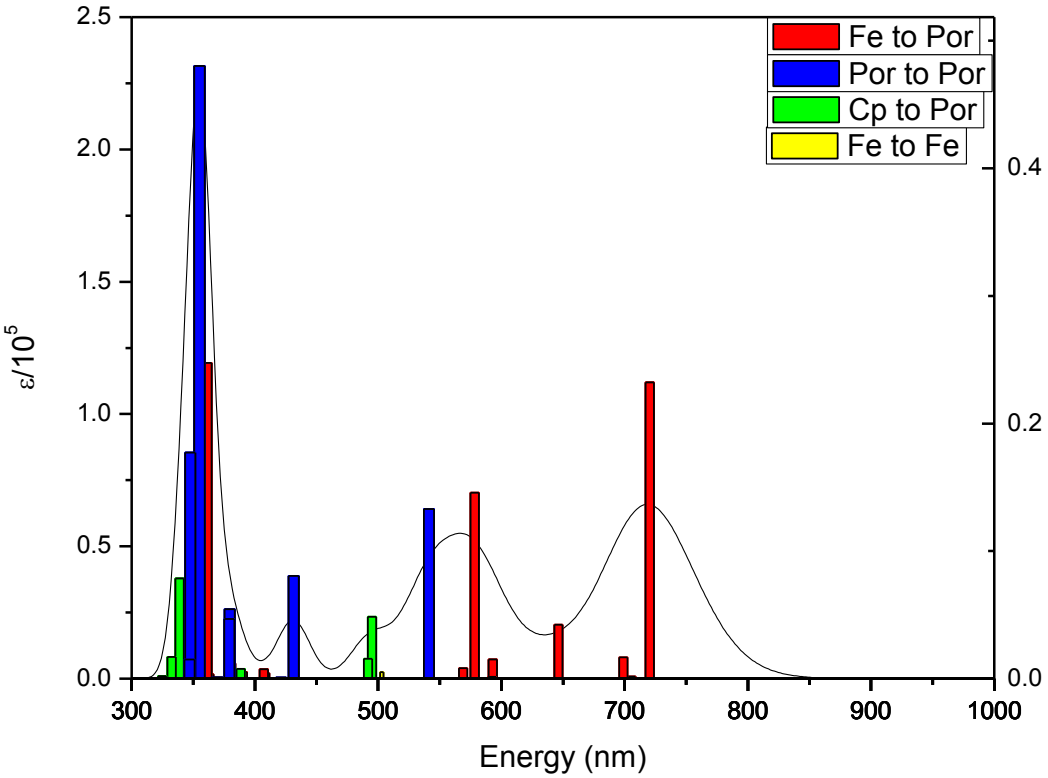


Figure 19a (TAP^{Fc}Mg) and 19b (TAP^{FcCN}Mg). Electronic structure plotted in terms of orbital contribution, or the percentage of a molectular orbital that is centered on a particular region or atom of the molecule. Cyclopentadieneyl group are shown in green, iron atoms are shown in blue, tetraazaporphyrin ring is shown in red, and magnesium atom is shown in black.

Figure 19 shows the composition of the molecular orbitals of TAP^{Fc}Mg (Figure 19a) and TAP^{FcCN}Mg (Figure 19b). Both compounds have degenerate LUMO and LUMO+1 orbitals that are dominantly tetraazaporphyrin centered (>80%). Higher energy unocupied orbitals are also heavily tetraazaporphyrin centered, but to slightly

lesser extents. Both compounds have HOMO to HOMO-7 orbitals comprised mainly of ferrocenyl character (mainly iron centered orbitals with some cyclopentadienyl centered area as well). It is not until HOMO-8 in both compounds that we begin to see increasing tetraazaporphyrin character and the π orbitals. Even then the HOMO-8 and neighboring orbitals are fairly mixed (~40% tetraazaporphyrin, ~60% ferrocene or ~10% iron and ~50% cyclopentadienyl). This analysis is partially consistent with Gouterman's four orbital model of porphyrins and related compounds[59, 60]. This model states that the LUMO and LUMO+1 orbitals are degenerate π* orbitals and the HOMO and HOMO-1 orbitals are almost degenerate π orbitals[61]. In our case, with ferrocene substituted tetraazaporphyrins, the HOMO orbitals of the ferrocene substituents lie between the HOMO-8 (π) and LUMO (π*) orbitals of the tetraazaporphyrin pushing the "HOMO" and "HOMO-1" orbitals described by Gouterman's model to the HOMO-8 and HOMO-9 levels.

With the electronic transitions already identified as part of the initial PCM-TDDFT calculations, they can now be separated by ground and excited orbital contribution (see Figures 20 and 21).


Fe to Por
Por to Por
Cp to Por
Fe to Fe
ε/10^5
Energy (nm)
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700
800
900
1000

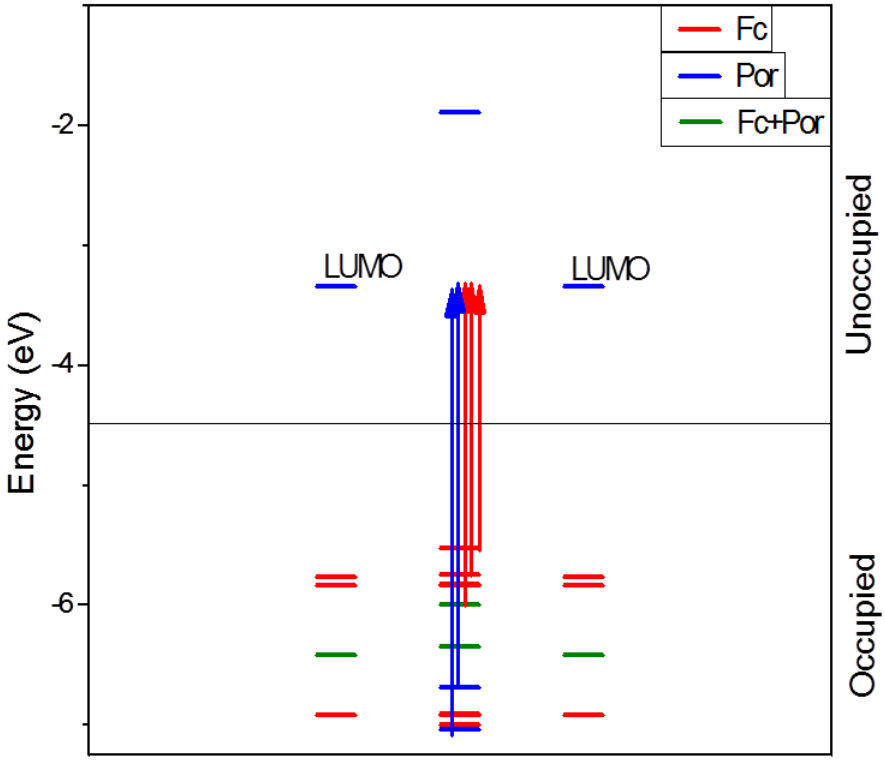
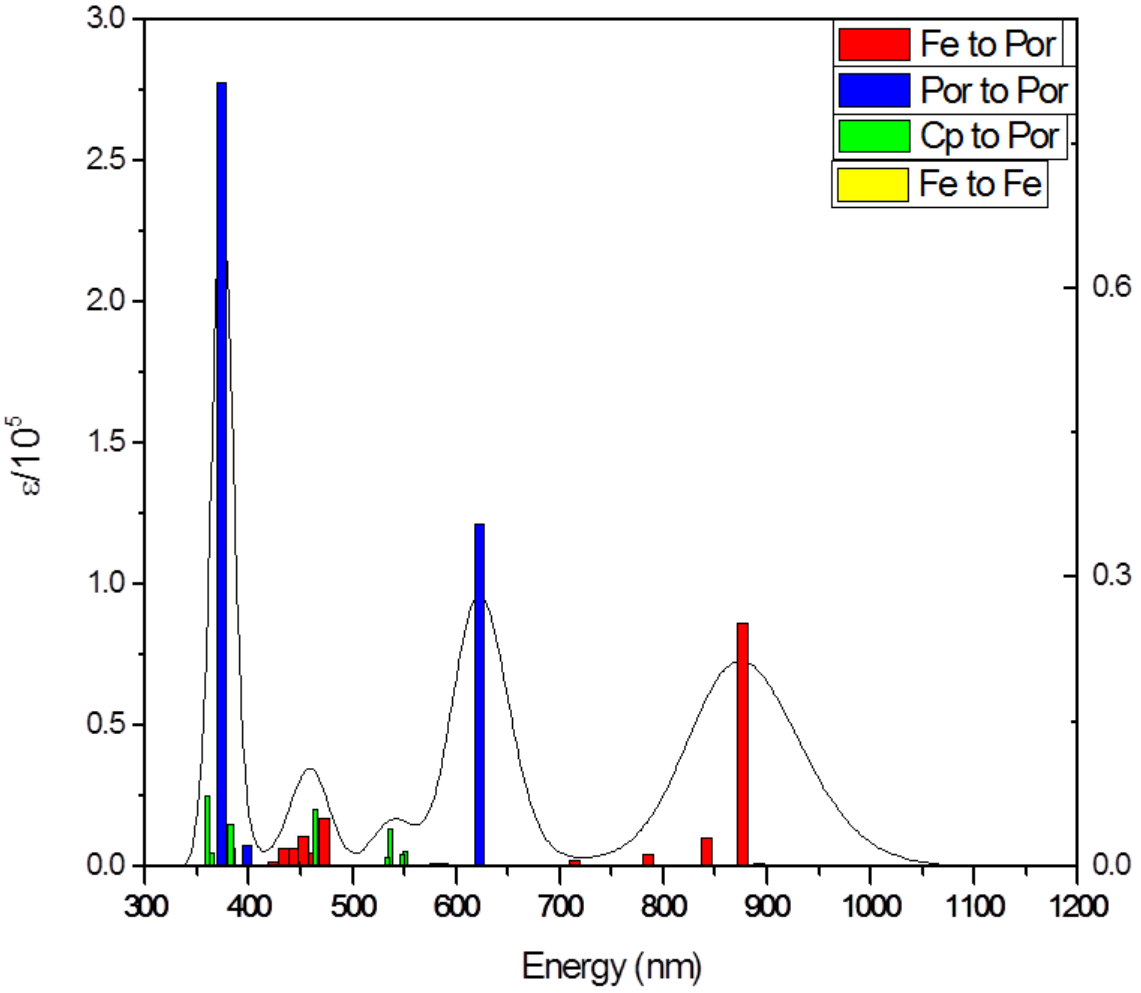


Figure 20a and 20b: TAP^{Fc}Mg PCM-TDDFT calculations are shown, separated by transition type. Iron to Tetraazaporphyrin in red, cyclopentadiene to tetraazaporphyrin in green (both charge transfer transitions), tetraazaporphyrin to tetraazaporphyrin in blue (π→π transitions), and iron to iron in yellow (while present, all of these transitions have very weak epsilon values and are not discussed). Energy diagram also shown. Each line represents a molecular orbital: tetraazaporphyrin based orbitals colored blue; ferrocenyl based orbitals colored red; heavily mixed orbitals colored green. Arrows represent the electronic transitions corresponding to the major peaks from PCM-TDDFT calculations and are color coordinated to transition type. The separations of the orbital lines indicate degeneracy. Orbital lines in the center column indicate singly degenerate orbitals. Doubly degenerate orbitals are shown separated out on the left and right columns.*


Fe to Por
Por to Por
Cp to Por
Fe to Fe
ε/10^5
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2.0
1.5
1.0
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0.0
0.6
0.3
0.0
300
400
500
600
700
800
900
1000
1100
1200
Energy (nm)

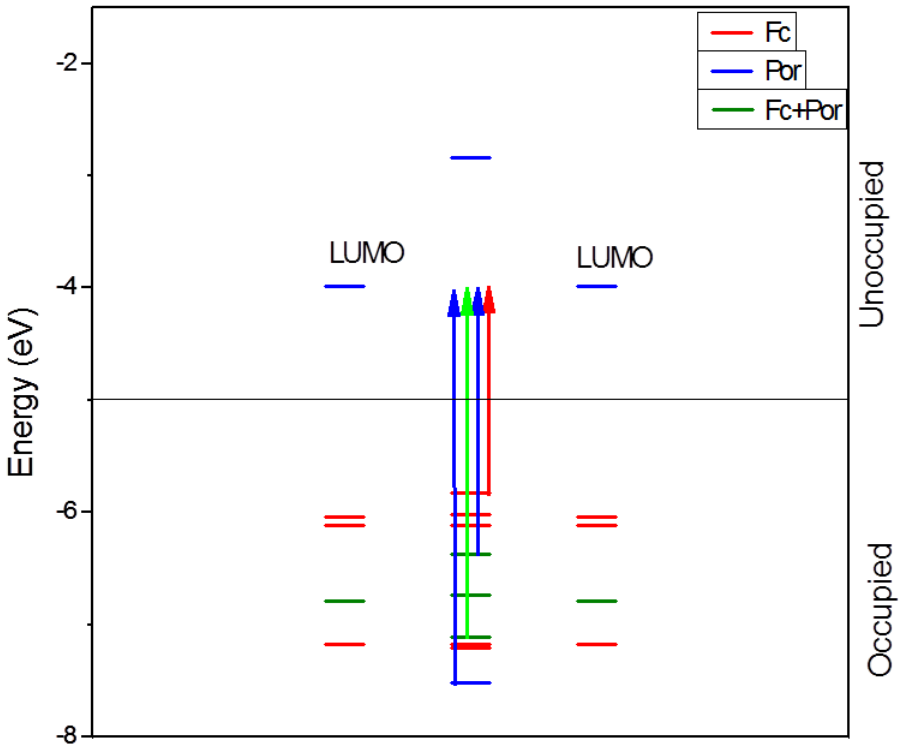
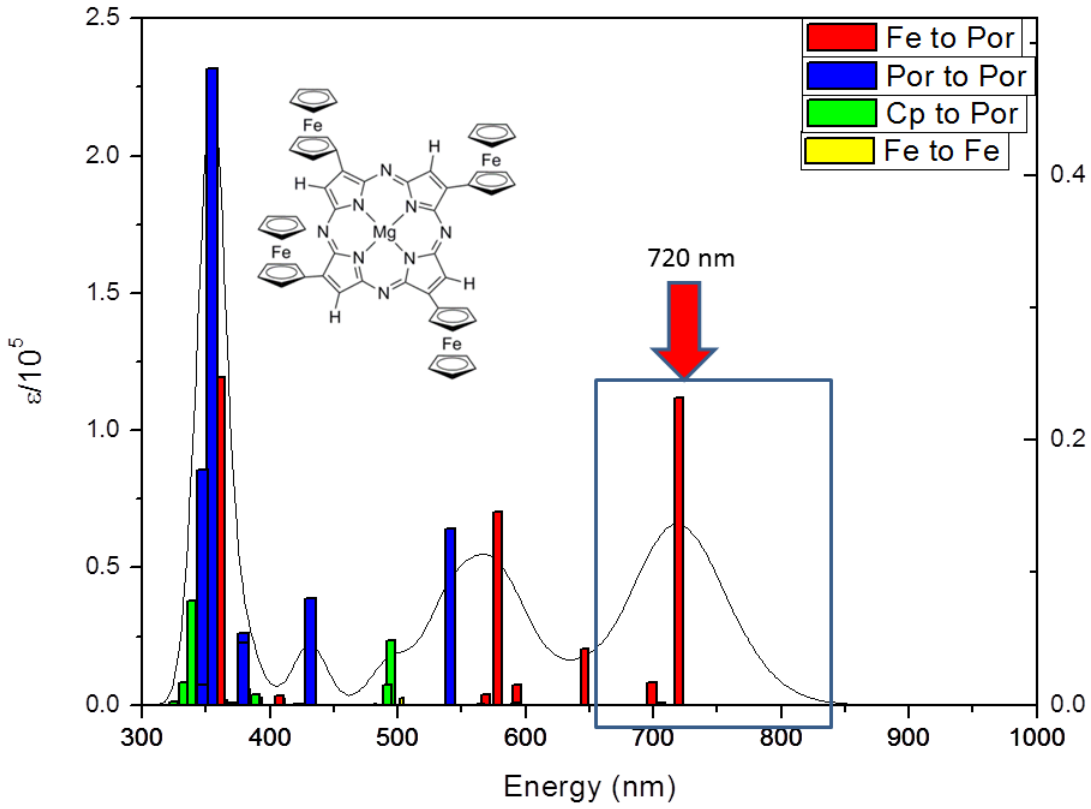


Figure 21a and 21b. TAP^{FcCN}Mg PCM-TDDFT calculations are shown, separated by transition type. Iron to Tetraazaporphyrin in red, cyclopentadiene to tetraazaporphyrin in green (both charge transfer transitions), tetraazaporphyrin to tetraazaporphyrin in blue (π→π transitions), and iron to iron in yellow (while present, all of these transitions have very weak epsilon values and are not discussed). Energy diagram also shown. Each line represents a molecular orbital: Tetraazaporphyrin based orbitals colored blue; ferrocenyl based orbitals colored red; heavily mixed orbitals colored green. Arrows represent the electronic transitions corresponding to the major peaks from PCM-TDDFT calculations and are color coordinated to transition type. The separations of the orbital lines indicate degeneracy. Orbital lines in the center column indicate singly degenerate orbitals. Doubly degenerate orbitals are shown separated out on the left and right columns.*

Initial analysis shows that we do have our two distinct types of transitions as initially theorized (the blue porphyrin to porphyrin transitions and the red iron to porphyrin transitions; green cyclopentadienyl to porphyrin are also present, but not as prominent in most transitons). However once the actual contribution is calculated and

analyzed, it is apparent that the transitions are not as specific as purely one type of transiton.

The PCM-TDDFT calculations show four major absorbance peaks on each spectrum, with each peak a result of one major electronic transition (two transitions in the case of the ~550 nm peak in the hydrogen substituted tetraazaporphyrin). With each one of these four (or five) electronic trasitions, the orbitals involved were calculated and generated. One thing in common with all of the major transitions to be discussed is that they are all degenerate transitions.



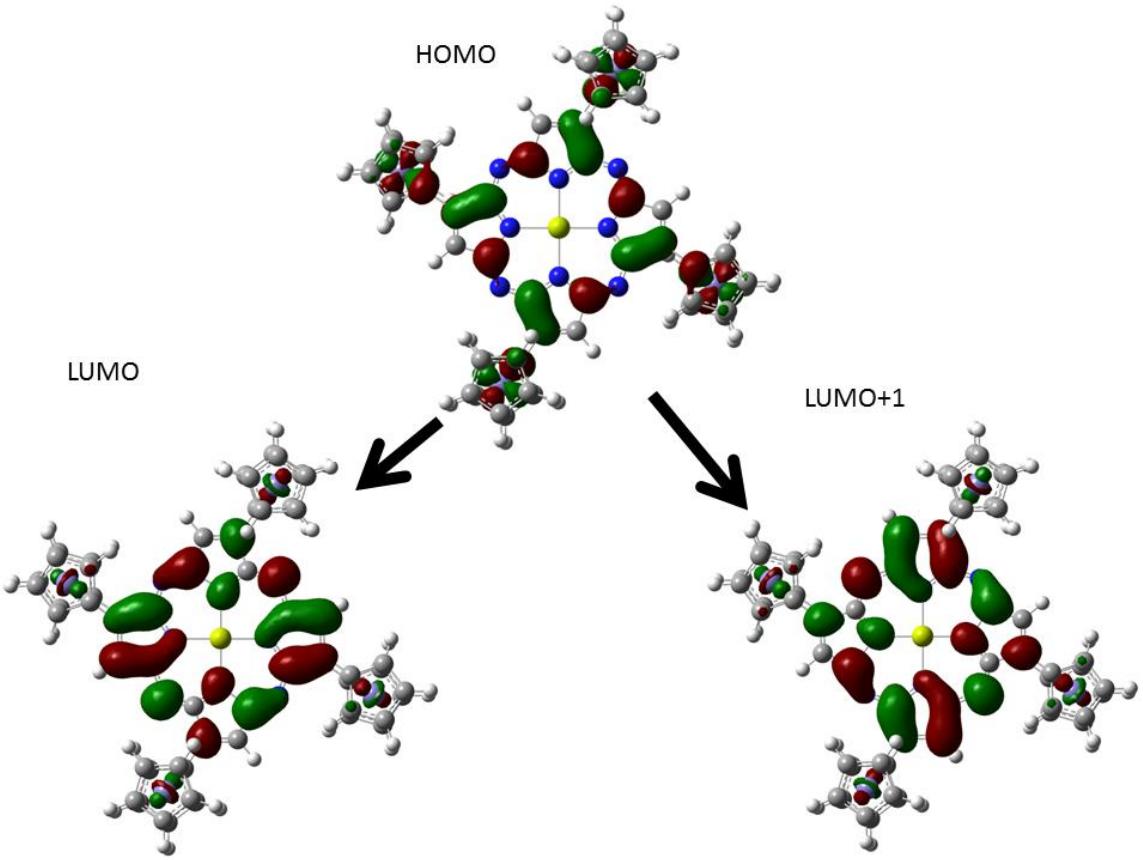
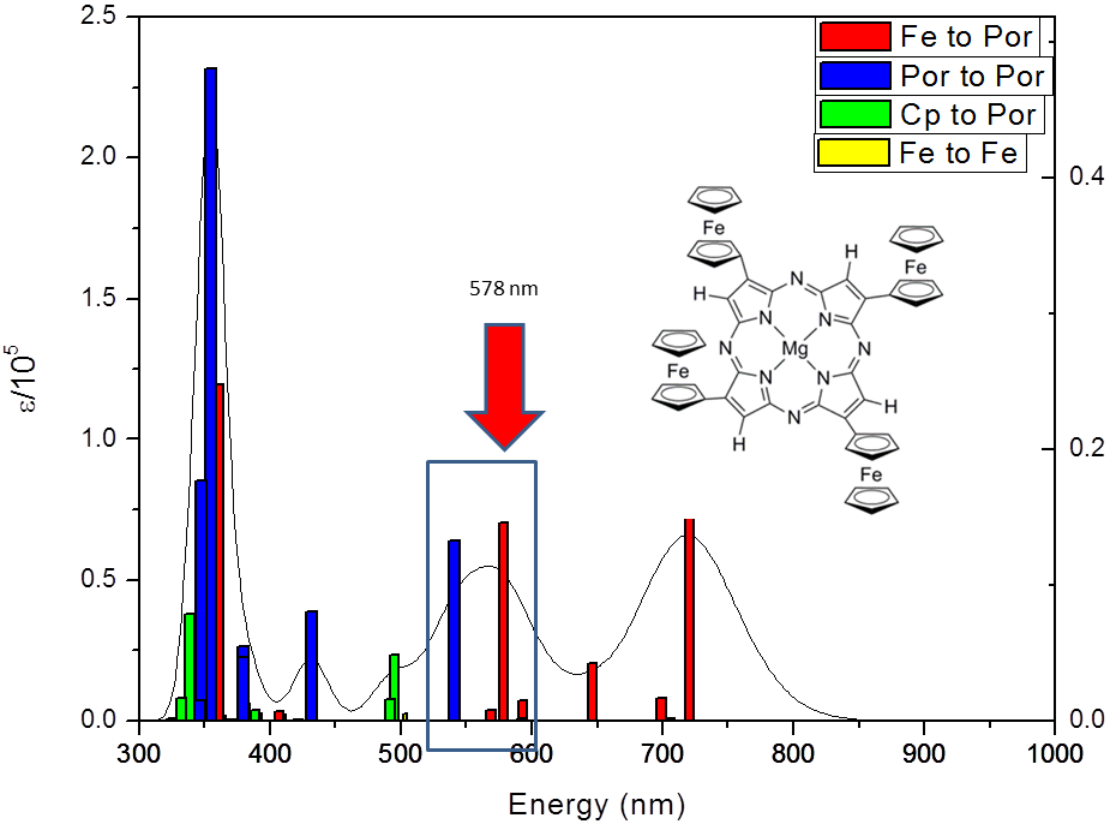


Figure 22a (Spectrum). Region 1 transition of TAP^{Fc}Mg. PCM-TDDFT calculated spectra with transition highlighted. Figure 22b. Corresponding orbital transition from HOMO level to degenerate LUMO and LUMO+1 levels.

Beginning with TAP^{Fc}Mg, the lowest energy major transition (identified in Figure 22) occurs with a relatively broad peak at 720 nm. This excited state is calculated to be mainly iron (HOMO) to tetraazaporphyrin (LUMO/LUMO+1) transition. However, the HOMO level is quite mixed showing some tetraazaporphyrin character (~25% TAP) coupled with the iron centered character of the orbital. The LUMO and LUMO+1 levels are easier to characterize being dominantly tetraazaporphyrin based in character. This would indicate that the transition, while predominately a charge transfer transition, has partial $\pi \rightarrow \pi^*$ character.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Cp to Por
Fe to Fe
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ε/10^5
Energy (nm)
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0.4
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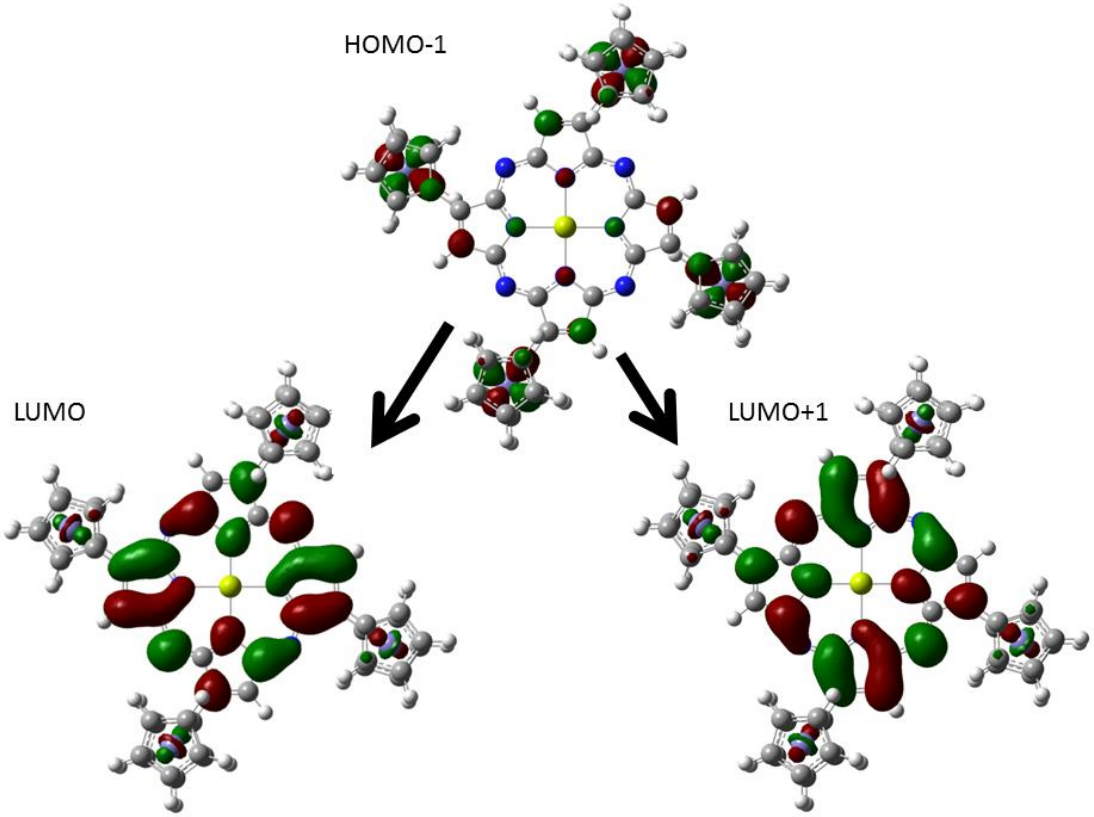
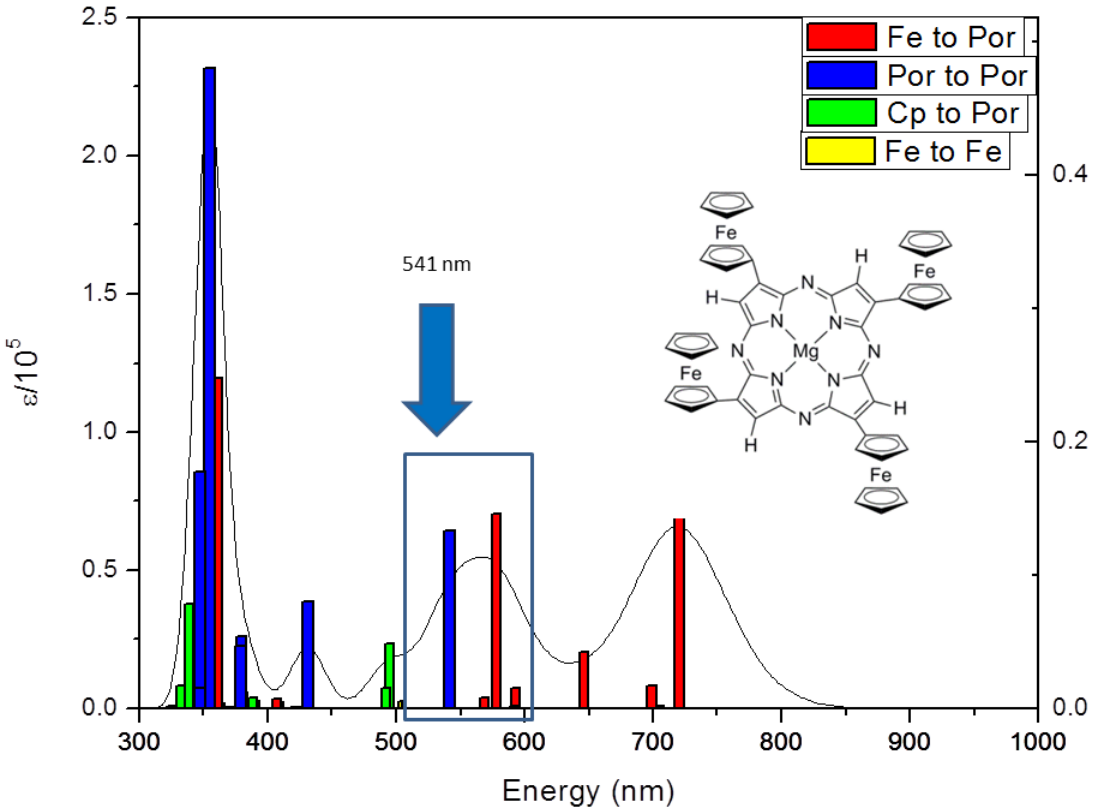


Figure 23a. Region 2 absorbance peak with transition highlighted. Figure 23b. corresponding orbital transition from HOMO-1 to degenerate LUMO and LUMO+1 levels.


Fe to Por
Por to Por
Cp to Por
Fe to Fe
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ε/10^5
Energy (nm)
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1.0
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0.0
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1000
Fe
Fe
Fe
Fe
Mg
N
H

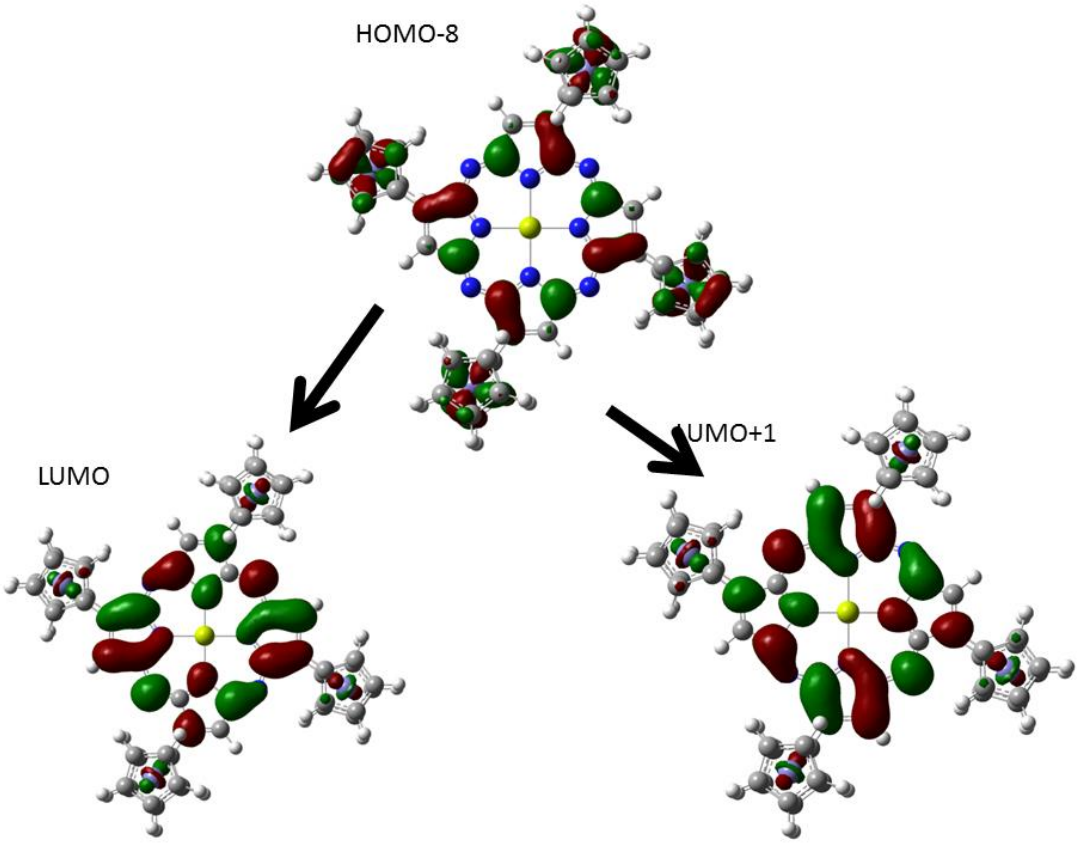
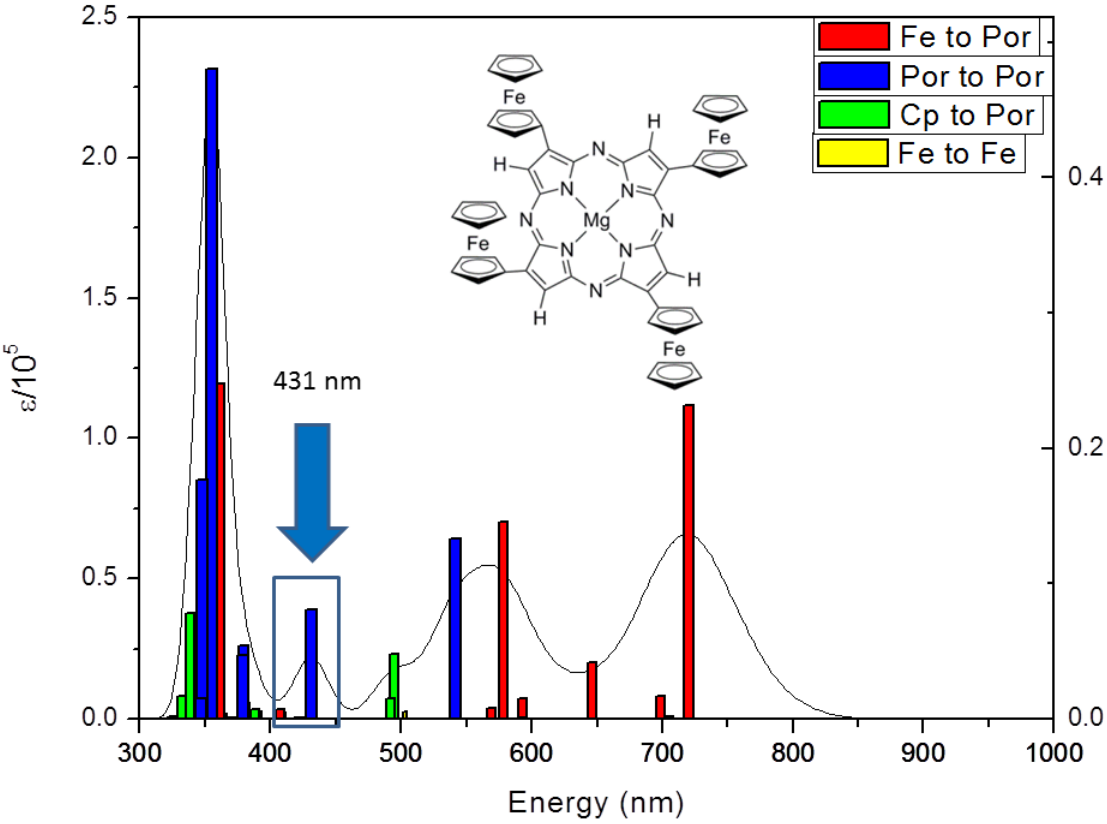


Figure 24a. 2nd Region 2 transition highlighted. Figure 24b. corresponding orbital transition from HOMO-8 to degenerate LUMO and LUMO+1 levels.

The second major energy absorption peak of $TAP^{Fc}Mg$ is centered at approximately 550 nm and actually consists of two transitions (shown in Figures 23 and 24), both charge transfer transitions. The lower energy transition in this region is again degenerate and occurs at 578 nm and corresponds to an excitation from the HOMO-1 level to LUMO and LUMO+1 levels. There is less mixed character than in the previous major transition with the HOMO-1 level being predominately iron based in character with some cyclopentadienyl character. This transition is clearly a charge transfer transition. The higher energy transition in this region occurs at 541 nm and predominately consists of the degenerate excitations from HOMO-8 level to

LUMO/LUMO+1 levels. The HOMO-8 level is fairly mixed with ~60% of the orbital centered on the tetraazaporphyrin ring and a significant contribution from the iron atoms in the ferrocene substituent. This results in the 541 nm transition being predominately a $\pi \rightarrow \pi^*$ transition with significant charge transfer character.



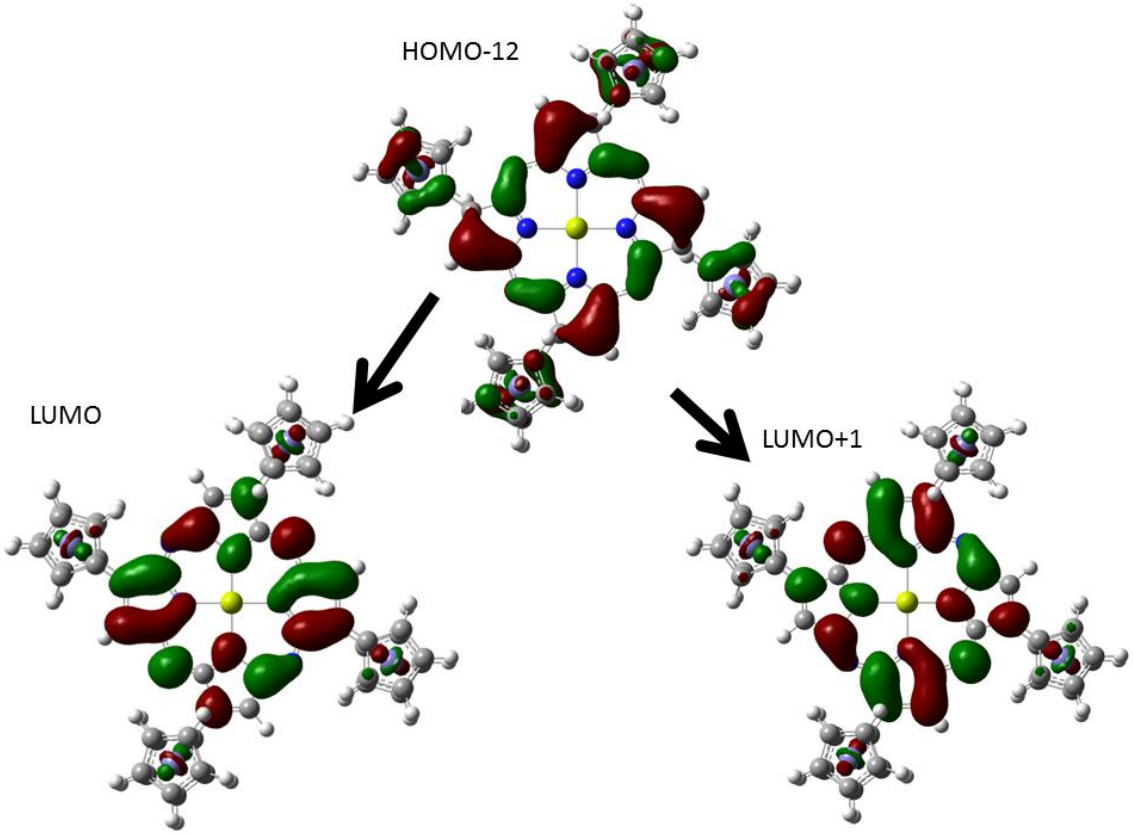
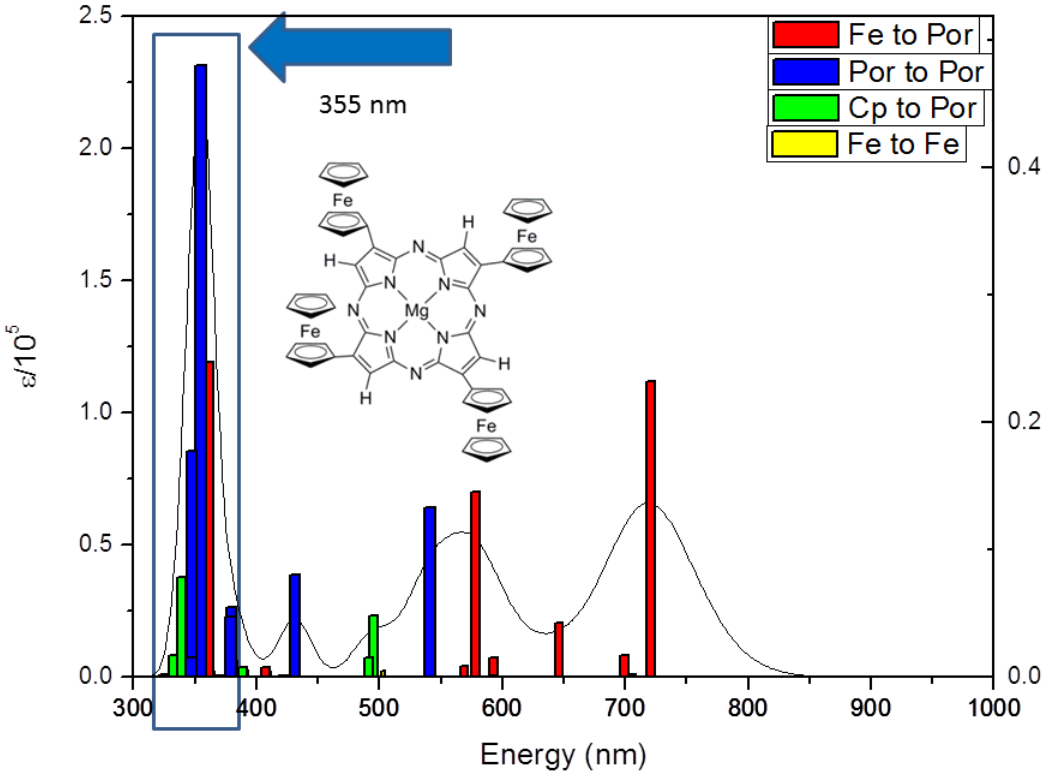


Figure 25a. Region 3 absorbance peak with transition highlighted. Figure 25b. corresponding orbital transition from HOMO-12 to degenerate LUMO and LUMO+1 levels.

Region 3 (identified in Figure 25) is only made up of one major transition, but does not show in the experimental spectrum due to the dominance of the following intense transition at 355 nm. This transition is also degenerate, comprised of excitations from the HOMO-12 level to LUMO/LUMO+1. The HOMO-12 orbital is dominant in tetraazaprophyrin centered character, but does include slight cyclopentadiene character (~60% TAP). This transition can be characterized as a predominately $\pi \rightarrow \pi^*$ transition, but with some charge transfer character included.


Fe to Por
Por to Por
Cp to Por
Fe to Fe
355 nm
ε/10^5
Energy (nm)
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2.0
1.5
1.0
0.5
0.0
0.4
0.2
0.0
300
400
500
600
700
800
900
1000
Fe
Mg
N
H

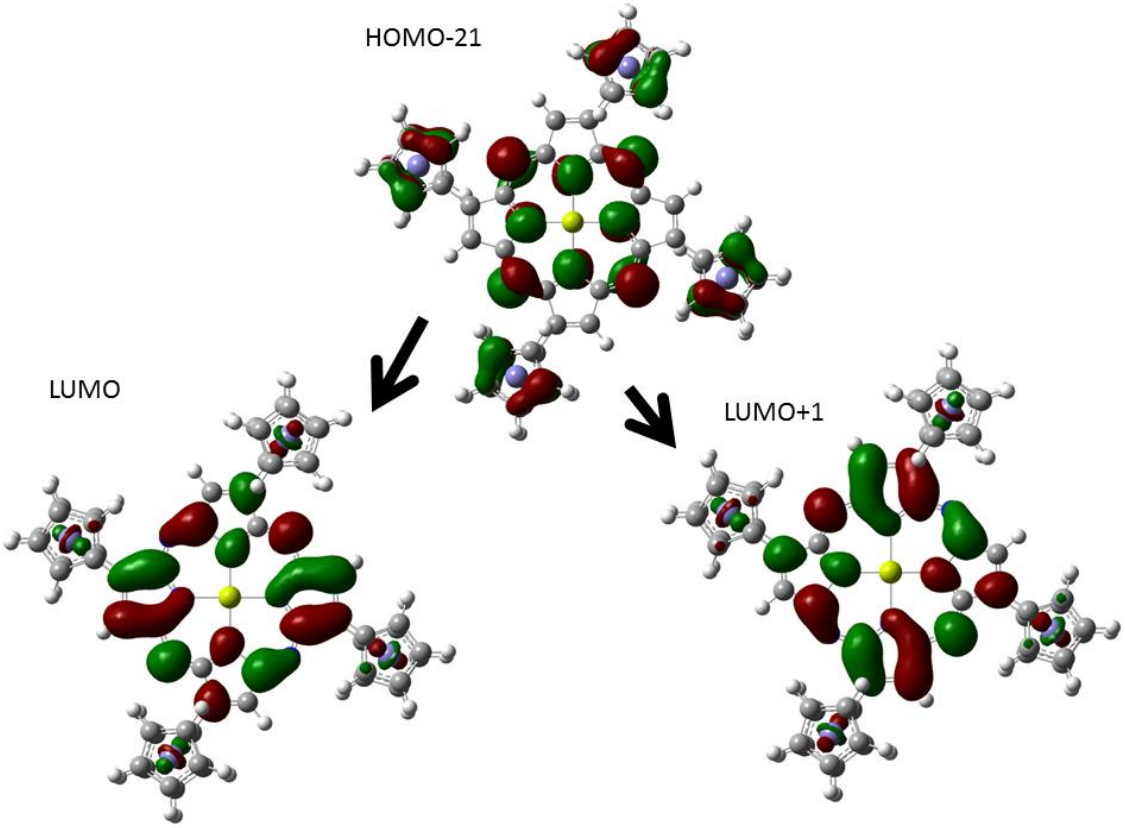
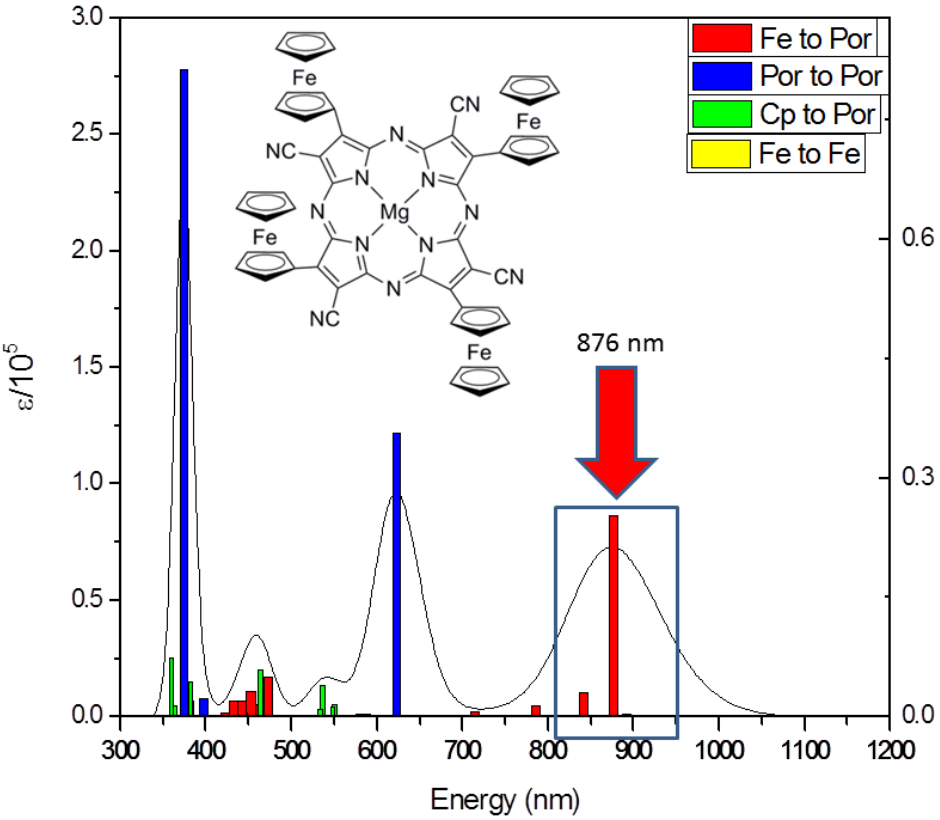


Figure 26a. Region 4 absorbance peak with transition highlighted. Figure 26b. corresponding orbital transition from HOMO-21 to degenerate LUMO and LUMO+1 levels.

The final major transition (shown in Figure 26) for TAP^{Fc}Mg occurs at 355 nm. Again degenerate, this transition arises from an excitation from the HOMO-21 level to the LUMO/LUMO+1 levels. The HOMO-21 level is rather complex in character. While the orbital is mostly tetraazaporphyrin in character, making the transition a $\pi \rightarrow \pi^*$ transition, there is a significant portion of the orbital that is centered on the ferrocene ligands (~45% Fc), making the charge transfer character of the transition also significant.


Fe to Por
Por to Por
Cp to Por
Fe to Fe
876 nm
ε/10^5
Energy (nm)
Fe
CN
NC
Mg
N

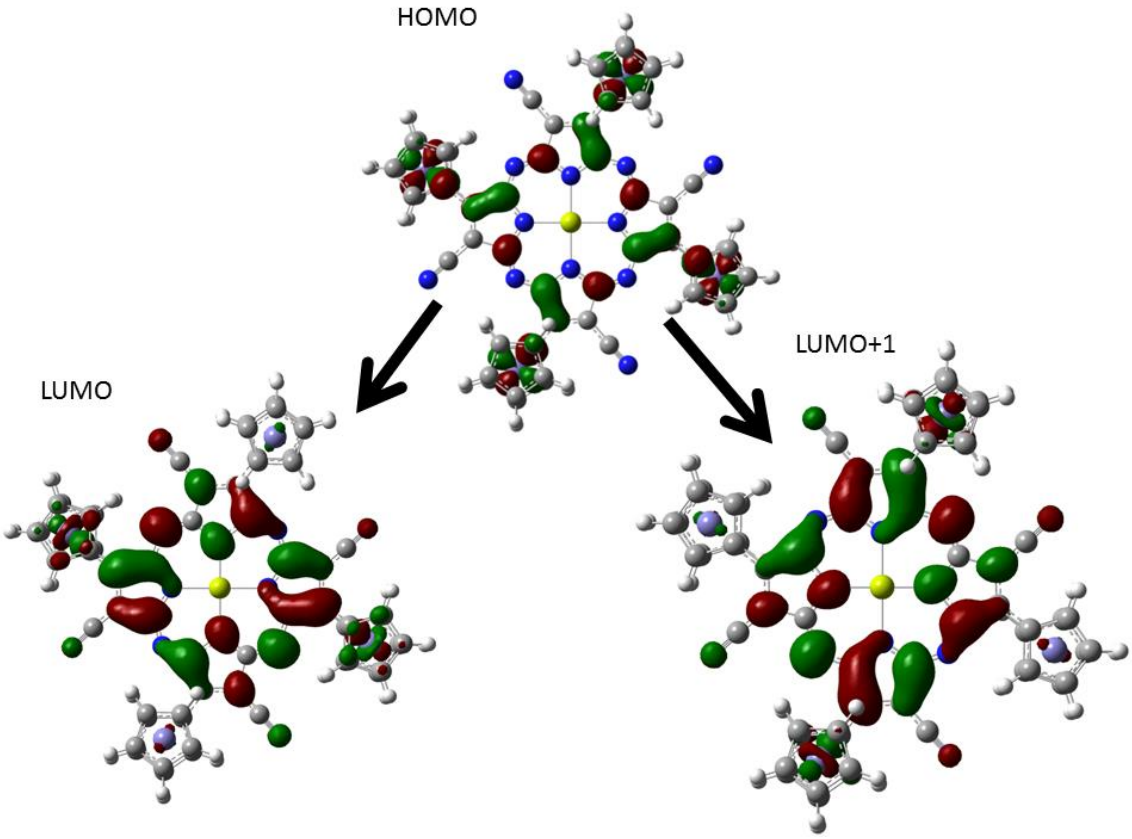
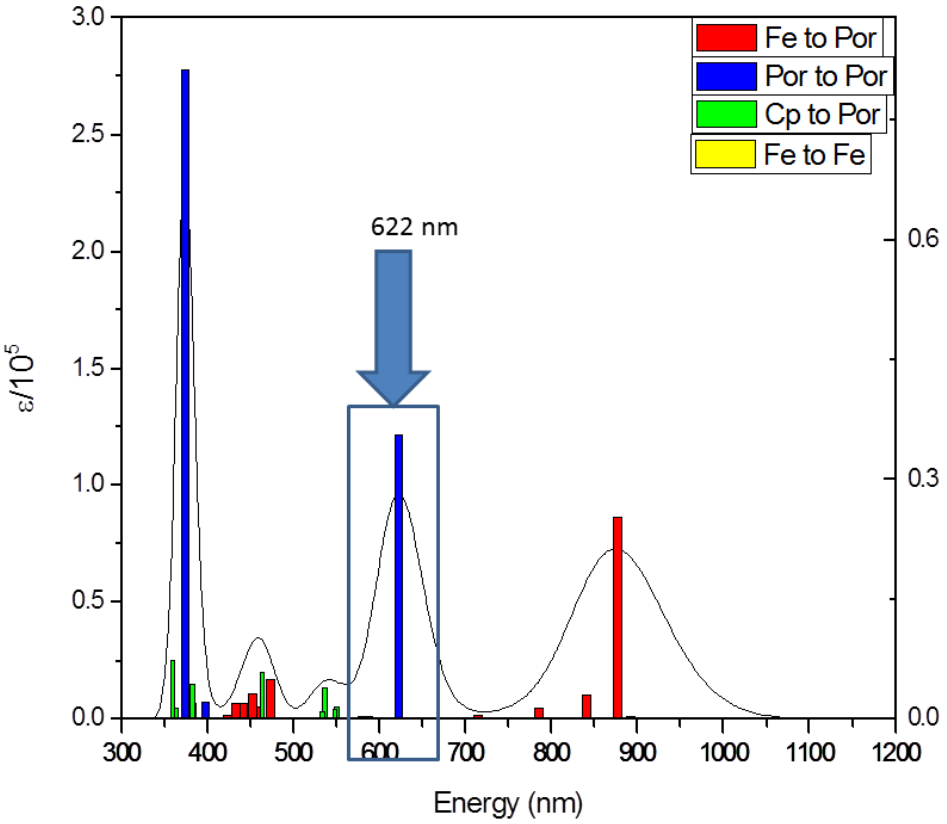


Figure 27a (Spectrum). Region 1 absoebance peak of TAP^{FcCN}Mg highlighted. PCM-TDDFT calculated spectra with transition highlighted. Figure 27b. Corresponding orbital transition from HOMO level to degenerate LUMO and LUMO+1 levels.

The lowest energy transition of TAP^{FcCN}Mg (shown in Figure 27) is similar to the non-cyanide substituted compound. Centered at 876 nm, it occurs from the degenerate transition of the HOMO to LUMO/LUMO+1 levels. Also like the non- cyanide substituted case, the HOMO level is mostly iron centered with some tetraazaporphyrin character (~25% TAP). The LUMO and LUMO+1 levels are again almost entirely porphyrin based in character. This makes this transition mostly a charge transfer transiton, but is also partly a $\pi \rightarrow \pi^*$ transition.


Fe to Por
Por to Por
Cp to Por
Fe to Fe
622 nm
ε/10^5
Energy (nm)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.6
0.3
0.0
300
400
500
600
700
800
900
1000
1100
1200

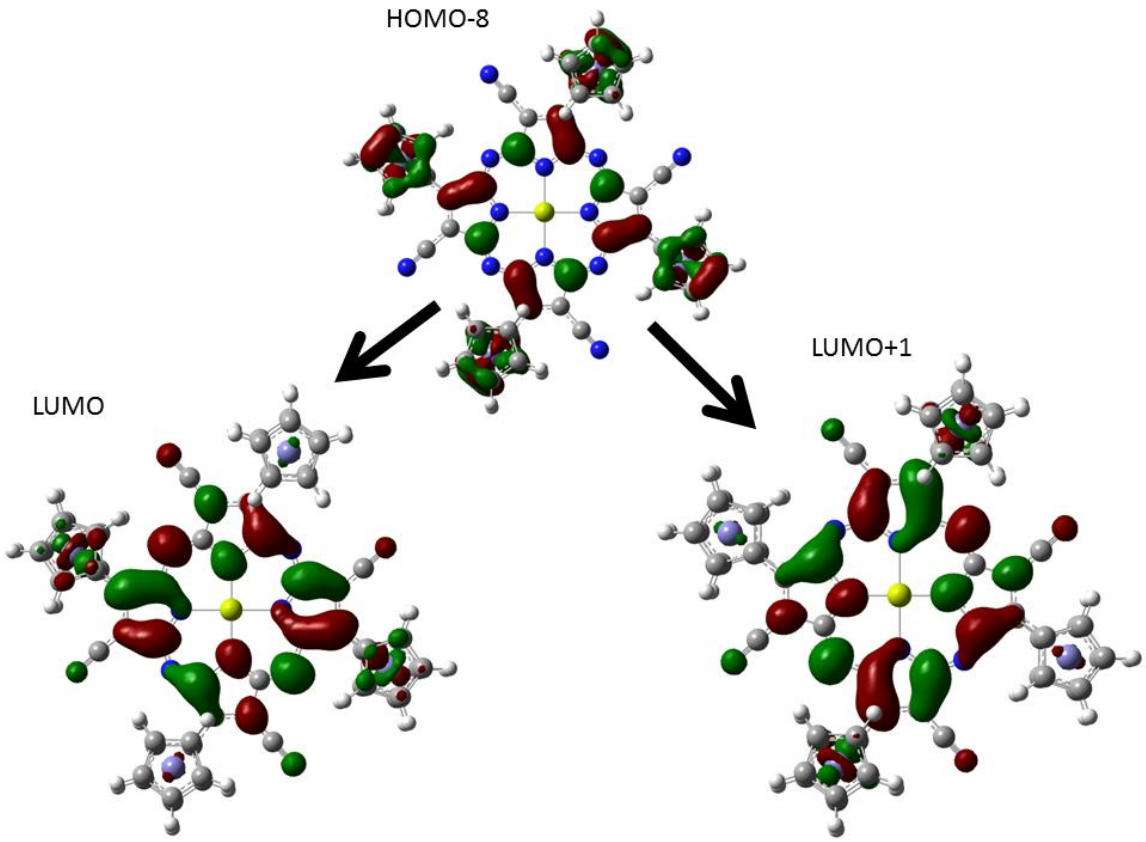
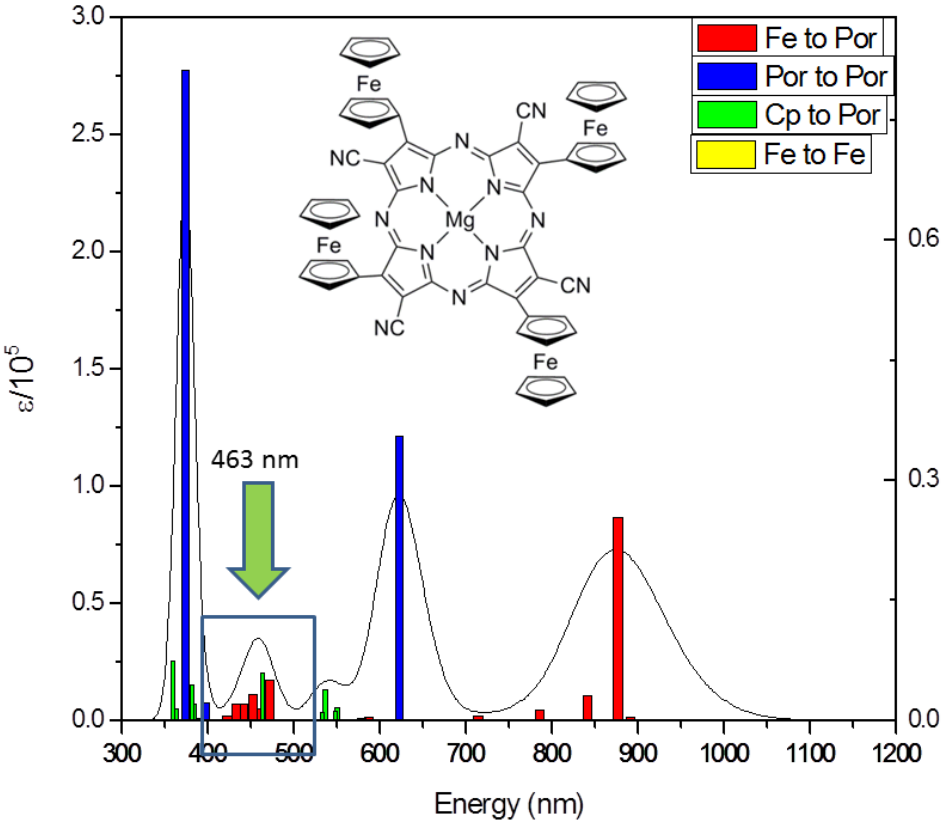


Figure 28a. Region 2 absorbance peak with transition highlighted. Figure 28b. corresponding orbital transition from HOMO-8 to degenerate LUMO and LUMO+1 levels.

The Region 2 transition (indicated in Figure 28) of TAP^{FcCN}Mg occurs at 622 nm. Like TAP^{Fc}Mg, it occurs from a transition from the HOMO-8 level to the degenerate LUMO/LUMO+1 levels. Like TAP^{Fc}Mg, the HOMO-8 level is again fairly mixed, but to a lesser extent. The tetraazaporphyrin ring makes up ~70% of the molecular orbital, with significant contribution from the iron atom. This makes the 622 nm transition mixed, with more $\pi \rightarrow \pi^*$ transition character than charge transfer character.


Fe to Por
Por to Por
Cp to Por
Fe to Fe
463 nm
ε/10^5
Energy (nm)
Fe
CN
NC
Mg
N
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.6
0.3
0.0
300
400
500
600
700
800
900
1000
1100
1200

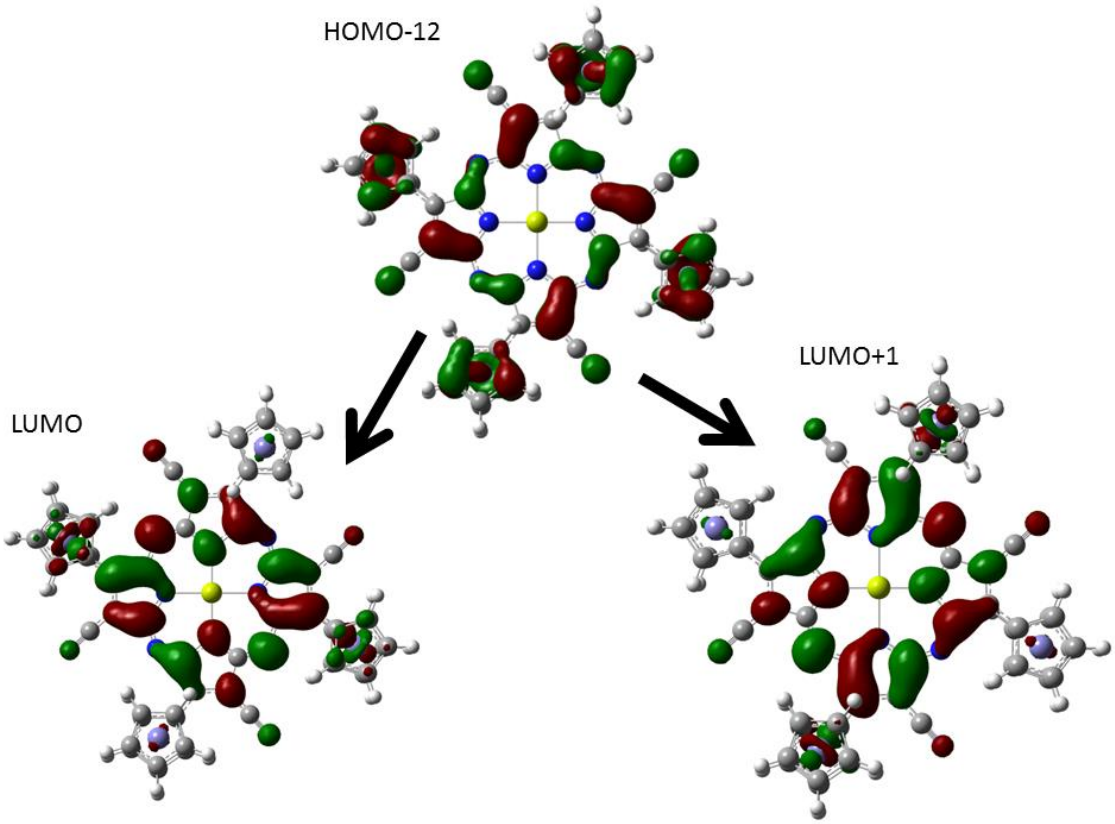
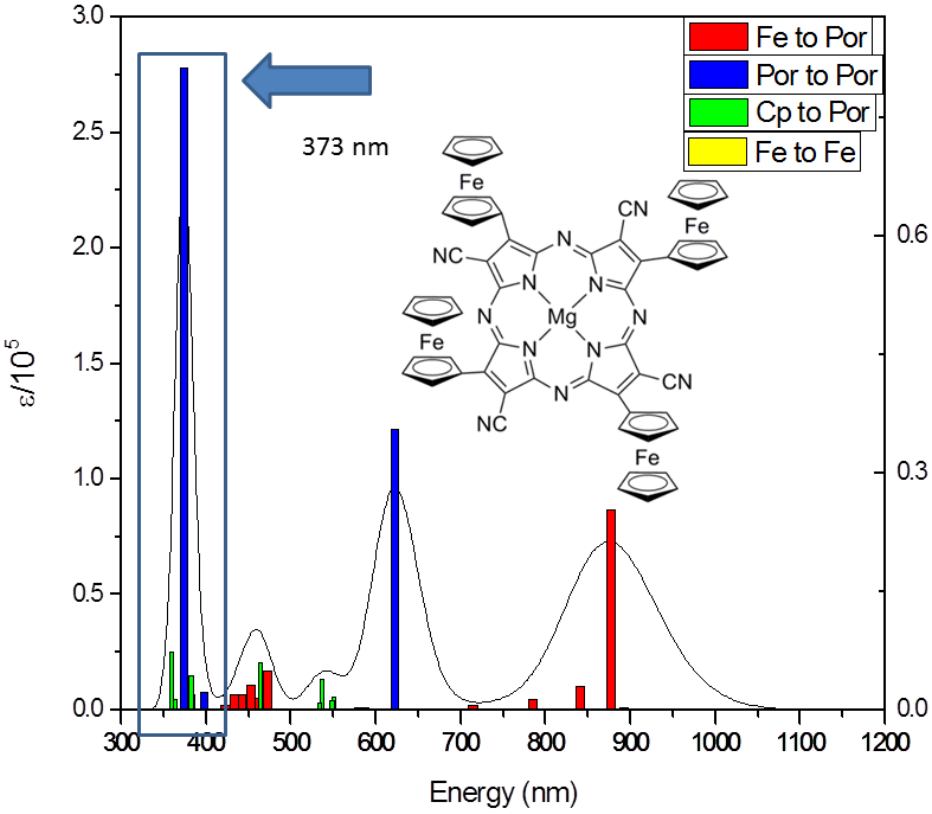


Figure 29a. Region 3 absorbance peak with transition highlighted. Figure 29b. corresponding orbital transition from HOMO-12 to degenerate LUMO and LUMO+1 levels.

The Region 3 absorbance peak (shown in Figure 29) is composed of multiple weak transitions. The strongest transition in this range occurs at 463 nm and is an excitation from the HOMO-12 level to the LUMO/LUMO+1 levels. The HOMO-12 level is another mixed character orbital (~40% TAP), with the majority of the orbital centered on the cyclopentadienyl rings and a small, but significant portion centered on the porphyrin ring. Despite the complex nature of this transition, it can be assigned as mostly a charge transfer transition, coupled with some slight $\pi \rightarrow \pi^*$ transition character.


Fe to Por
Por to Por
Cp to Por
Fe to Fe
373 nm
Fe
CN
Fe
NC
N
N
N
Mg
N
N
N
Fe
N
CN
NC
Fe
ε/10^5
Energy (nm)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0.0
0.3
0.6
300
400
500
600
700
800
900
1000
1100
1200

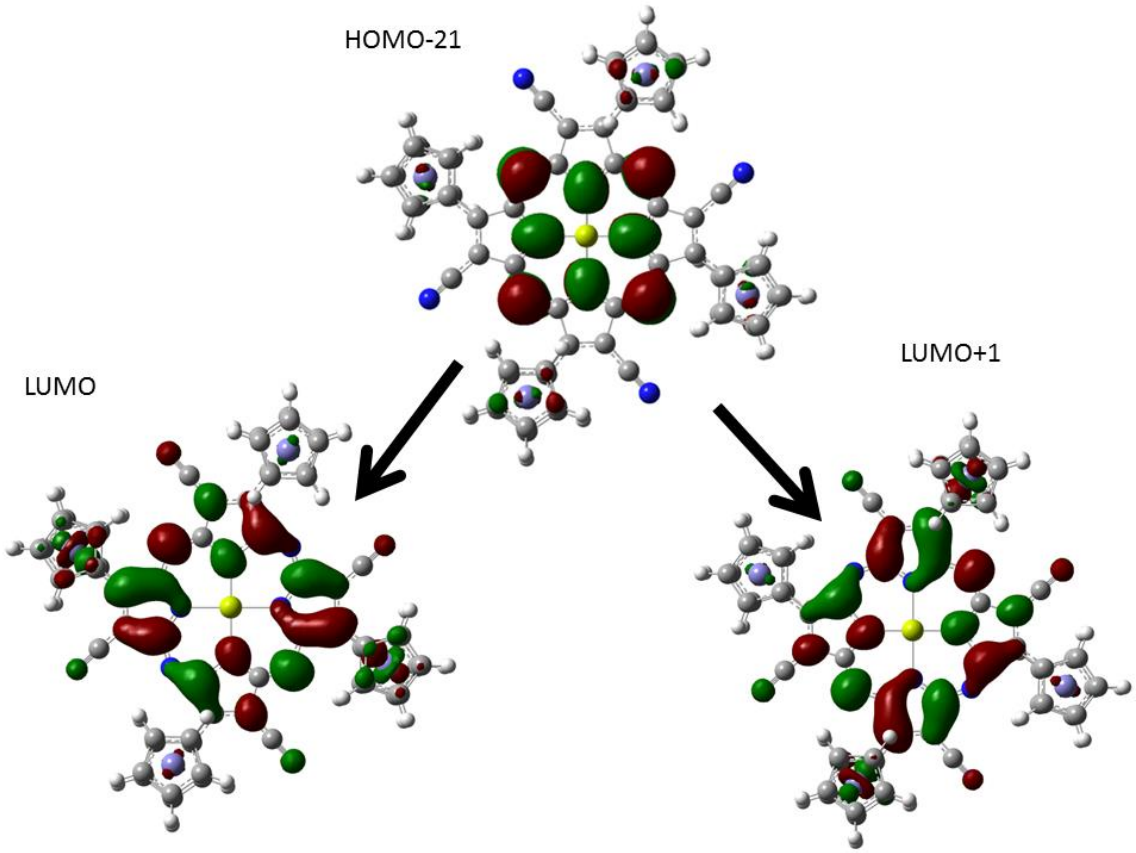


Figure 30a. Region 4 absorbance peak with transition highlighted. Figure 30b. corresponding orbital transition from HOMO-21 to degenerate LUMO and LUMO+1 levels.

The Region 4 absorbance peak (see Figure 30) consists of a single very intense transition that occurs at 373 nm. This transition is made up of an excitation from the HOMO-21 level to the LUMO/LUMO+1 levels. The character of the HOMO-21 level is relatively easier to characterize being almost exclusively porphyrin character. Combined with the pophyrin character of the LUMO and LUMO+1 levels, this transition can be assigned as being a $\pi \rightarrow \pi^*$ transition with no significant amount of mixed character.

Discussion:

Using the B3LYP functional (~20% HF exchange), the major absorbance peaks shifted, from experiment to theory, from 13850 to 13888 cm^{-1}, 17331 to 17699 cm^{-1}, and 27548 to 28248 cm^{-1} for $TAP^{Fc}Mg$, and 11173 to 11415 cm^{-1}, 16051 to 16077 cm^{-1}, and 26109 to 26737 cm^{-1}. With the largest difference between theoretical and experimental peak locations being 700 cm^{-1}, this gave the best agreement between theory and experiment, providing acceptable estimations for both charge transfer and $\pi \rightarrow \pi^*$ electronic transitions.

Because of this agreement, further analysis was calculated using the B3LYP functional to determine electronic structure and assign electronic transitions. The electronic structure of $TAP^{Fc}Mg$ was calculated to have degenerate LUMO and LUMO+1 levels that have heavy tetraazaporphyrin character (~90% TAP) and a HOMO level that is predominately ferrocene in character with some tetraazaporphyrin character mixed in (~40% TAP). Lower occupied orbitals maintain ferrocene character (<10% TAP) until HOMO-8 to HOMO-12 which are fairly mixed character orbitals (between 35% and 60% TAP). The electronic structure of $TAP^{FcCN}Mg$ was also calculated to have degenerate LUMO and LUMO+1 levels that are heavily tetraazaporphyrin in character (~85% TAP) and a HOMO level that is slightly tetraazaporphyrin mixed with mostly ferrecene character (~25% TAP). Lower orbital levels are also predominately ferroecene characterized orbitals with less that 10% tetraazaporphyrin character mixed in until HOMO-8. Again, HOMO-8 to HOMO-12 levels consist of fairly mixed orbitals containing between 35 and 40% tetraazaporphyrin character.

Returning to our original desire to look for cheap and efficient dyes for use in DSSC, it would seem that the discussed ferrocene substituted tetraazaporphyrins would be good candidates for antenna compounds in DSSC. These two compounds could potentially improve on what has been previously achieved using ruthenium and porphyrin based dyes. Ruthenium dyes operate using charge transfer electronic transitions. These transitions led to very intense absorbance peaks in the UV region, but did not absorb much past 700 or 800 nm. Since the solar spectrum emits past 2000 nm, this leaves over half of the solar spectrum to not be absorbed by ruthenium based dyes. Also, due to the limited nature of elemental ruthenium as a source for synthesis, ruthenium based dyes can become quite expensive, which would limit widespread adoption of solar cells made from these dyes. Porphyrin based dyes operate using $\pi \rightarrow \pi^*$ electronic transitions. These trasitions also lead to intense absorption peaks in the UV region, as well as some absorbance into the IR range, but again do not absorb much past 700 or 800 nm. Porphyrins are more attractive as a compound since their precursor compounds for synthesis are readily available at low cost, compared to ruthenium and ruthenium based dyes. Also, the solar power conversion efficiency of porphyrins and related compounds has been increasing greatly over the past two decades. In fact, the solar power conversion efficiency of porphyrins has increased so much that porphyrin based compounds used in DSSC could soon rival the efficiencies of other inorganic thin film technologies.

The tetraazaporphyrins were designed to potentially include both charge transfer and $\pi \rightarrow \pi^*$ electronic transitions to combine the benefits of ruthenium and porphyrin based dyes. The calculations conducted through this research confirmed that both charge

transfer and π→π* electronic transitions were present, although achieved by containing transitions that were of mixed character rather than transitions that were purely charge transfer or π→π* transitions. By including both charge transfer and π→π* transitions, absorbance gaps were minimized and a fairly large absorbance range was observed. However, there are still some problems keeping these compounds from being perfect solar antennas. Both compounds absorb poorly around 500 nm; as shown in Figure 7, this is the area with the strongest emission of the solar spectrum. Also, $TAP^{Fc}Mg$ does not absorb past 1000 nm, while $TAP^{FcCN}Mg$ does not absorb past 1200 nm. Again referring to Figure 7, this is only about half of the solar emission spectrum which emits until about 2000 nm.

In order to potentially fix these two problems, we should look at the difference between the absorbance spectrum of the two compounds as well as the Region 1 and Region 4 (and possibly Region 3) absorbance peaks (refer to Figure 12). The inclusion of the cyano group (an electronegative substituent) to the tetraazaporphyrin ring causes a slight red shift in the absorbance spectrum from $TAP^{Fc}Mg$ to $TAP^{FcCN}Mg$. There is a slight shift in the high energy Region 4 peak ($TAP^{Fc}Mg$: 363 nm; $TAP^{FcCN}Mg$: 383 nm). Creating a compound with a greater red shift with regard to this Region 4 peak (or possibly creating a more intense Region 3 peak) could help fill in the weak absorbance area around 500 nm. The red shift is much more noticeable in the low energy Region 1 peak ($TAP^{Fc}Mg$: 722 nm; $TAP^{FcCN}MG$: 895 nm). The Region 1 peak is also much broader in $TAP^{FcCN}Mg$ than the Region 1 peak in $TAP^{Fc}Mg$. A possible future research project would be to synthesize and analyze ferrocene substituted tetraazaporphyrins with different (possibly very electronegative) substituents placed in the beta positions where

the hydrogen or cyano groups are currently substituted on the tetraazaporphyrin ring. By varying the second substituent, we could see any possible effects on the Region 1 peak to see if it shifts further into the infrared region.

Conclusion:

The electronic structures of the two tetraazaporphyrins ($TAP^{Fc}Mg$ and $TAP^{FcCN}Mg$) were calculated leading to the transitions that make up UV-Vis-NIR spectra of these two compounds being fully analyzed. The spectra were analyzed based on a series of computational calculations using different levels of theory to find the best agreement between theory and experiment. The best agreement came from using the B3LYP hybrid functional, containing ~20% of HF exchange. The B3LYP functional was then used again for single point calculations used to assign the electronic transitions and generate molecular orbital contours. From the assignment, the lower energy transitions, as in Region 1 of both spectra, were found to be predominately MLCT in character resulting from transitions between the iron atoms and tetraazaporphyrin ring. The higher energy transitions, as in Region 4 of both spectra, were found to be predominately $\pi \rightarrow \pi^*$ transitions resulting from electronic excitations within the tetraazaporphyrin ring. The analysis also found that the major transitions, as explained in detail in the results of this thesis, were fairly mixed in character due to the mixed nature of the involved molecular orbitals, with predominately MLCT transitions containing a significant percentage of $\pi \rightarrow \pi^*$ transitions character and vice versa. While both types of transitions are present as expected, the real life scenario of the transitions being of mixed character is slightly more

complex than the initial hypothesis of a compound that contains a set of pure MLCT and $\pi \rightarrow \pi^*$ transitions.

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Appendix I: Supplemental Information:

Table S1: Vertical excitation energies of $TAP^{Fc}Mg$ using BPW91 PCM-TDDFT

Excited State 1: Singlet-E 0.8648 eV 1433.75 nm f=0.0070 <S**2>=0.000
245 ->250 0.22540
248 ->250 0.42887
249 ->250 0.42612
249 ->251 -0.25228
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3090.56395738
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-E 0.8648 eV 1433.74 nm f=0.0070 <S**2>=0.000
245 ->251 -0.22543
248 ->251 0.42886
249 ->250 -0.25229
249 ->251 -0.42611

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 0.8792 eV 1410.27 nm f=0.0000 <S**2>=0.000
246 ->251 -0.49204
247 ->250 0.49208

Excited state symmetry could not be determined.
Excited State 4: Singlet-?Sym 0.8828 eV 1404.47 nm f=0.0000 <S**2>=0.000
246 ->250 0.31657
246 ->251 0.37416
247 ->250 0.37403
247 ->251 -0.31687

Excited State 5: Singlet-E 0.8833 eV 1403.58 nm f=0.0010 <S**2>=0.000
244 ->250 0.22730
244 ->251 -0.16569
245 ->250 -0.36878
245 ->251 0.40001
248 ->251 0.33992

Excited State 6: Singlet-E 0.8833 eV 1403.58 nm f=0.0010 <S**2>=0.000
244 ->250 0.16567
244 ->251 0.22729
245 ->250 0.40006
245 ->251 0.36880
248 ->250 -0.33986

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 0.8854 eV 1400.34 nm f=0.0000 <S**2>=0.000
242 ->250 -0.14940
243 ->251 -0.14918
246 ->250 0.46950
247 ->251 0.46882

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 0.8874 eV 1397.17 nm f=0.0002 <S**2>=0.000
242 ->250 0.19179
243 ->251 -0.19196
246 ->250 -0.36560
246 ->251 0.27498
247 ->250 0.27512
247 ->251 0.36620

Excited State 9: Singlet-E 0.8878 eV 1396.58 nm f=0.0019 <S**2>=0.000
244 ->250 0.47872
244 ->251 0.24006
245 ->250 -0.20713
245 ->251 -0.30637
248 ->250 -0.18314
248 ->251 -0.11063
249 ->250 0.14516

Excited State 10: Singlet-E 0.8878 eV 1396.58 nm f=0.0019 <S**2>=0.000
244 ->250 -0.24004
244 ->251 0.47872
245 ->250 -0.30639
245 ->251 0.20717
248 ->250 0.11062
248 ->251 -0.18308
249 ->251 -0.14517

Excited state symmetry could not be determined.
Excited State 11: Singlet-?Sym 0.9107 eV 1361.47 nm f=0.0000 <S**2>=0.000
242 ->251 0.49767
243 ->250 -0.49765

Excited state symmetry could not be determined.
Excited State 12: Singlet-?Sym 0.9199 eV 1347.78 nm f=0.0000 <S**2>=0.000
242 ->250 0.12353
242 ->251 0.47781
243 ->250 0.47783
243 ->251 -0.12350

Excited State 13: Singlet-E 1.0331 eV 1200.08 nm f=0.1814 <S**2>=0.000
244 ->250 -0.34692
248 ->250 -0.36903
248 ->251 0.12375
249 ->250 0.44486

Excited State 14: Singlet-E 1.0331 eV 1200.07 nm f=0.1815 <S**2>=0.000
244 ->251 0.34691
248 ->250 0.12376
248 ->251 0.36902
249 ->251 0.44487

Excited state symmetry could not be determined.
Excited State 15: Singlet-?Sym 1.0427 eV 1189.06 nm f=0.0222 <S**2>=0.000
242 ->250 -0.43941
243 ->251 0.43950
246 ->250 -0.11761
246 ->251 0.17059
247 ->250 0.17060
247 ->251 0.11764

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 1.1014 eV 1125.69 nm f=0.0000 <S**2>=0.000
242 ->250 0.46532
243 ->251 0.46524
246 ->250 0.14602
247 ->251 0.14598

Excited State 17: Singlet-E 1.2944 eV 957.83 nm f=0.0020 <S**2>=0.000
240 ->250 0.47387
241 ->250 0.50953

Excited State 18: Singlet-E 1.2944 eV 957.83 nm f=0.0020 <S**2>=0.000
240 ->251 -0.47390
241 ->251 0.50950

Excited state symmetry could not be determined.
Excited State 19: Singlet-?Sym 1.2991 eV 954.38 nm f=0.0000 <S**2>=0.000
238 ->251 0.49223
239 ->250 0.49237

Excited state symmetry could not be determined.
Excited State 20: Singlet-?Sym 1.3002 eV 953.54 nm f=0.0000 <S**2>=0.000
238 ->251 0.49337

239 ->250 -0.49323

Excited State 21: Singlet-E 1.3295 eV 932.56 nm f=0.0296 <S**2>=0.000
240 ->250 0.50415
240 ->251 -0.11076
241 ->250 -0.46924

Excited State 22: Singlet-E 1.3295 eV 932.56 nm f=0.0296 <S**2>=0.000
240 ->250 0.11076
240 ->251 0.50412
241 ->251 0.46927

Excited state symmetry could not be determined.
Excited State 23: Singlet-?Sym 1.3334 eV 929.86 nm f=0.0031 <S**2>=0.000
238 ->250 0.49048
239 ->251 0.49093

Excited state symmetry could not be determined.
Excited State 24: Singlet-?Sym 1.3418 eV 924.02 nm f=0.0000 <S**2>=0.000
238 ->250 0.48396
239 ->251 -0.48351

Excited State 25: Singlet-E 1.9611 eV 632.23 nm f=0.1945 <S**2>=0.000
229 ->250 0.11866
232 ->251 0.14675
236 ->251 0.16655
237 ->251 0.60096
243 ->252 -0.17734
247 ->252 -0.10633

Excited State 26: Singlet-E 1.9611 eV 632.23 nm f=0.1944 <S**2>=0.000
229 ->251 -0.11866
232 ->250 0.14675
236 ->250 -0.16655
237 ->250 0.60096
242 ->252 0.17734
246 ->252 0.10631

Excited State 27: Singlet-B 1.9816 eV 625.69 nm f=0.0119 <S**2>=0.000
234 ->250 0.11306
235 ->251 -0.11301
245 ->252 0.27406
249 ->252 0.62533

Excited State 28: Singlet-A 1.9935 eV 621.95 nm f=0.0000 <S**2>=0.000

244 ->252 -0.43742
248 ->252 0.54897

Excited State 29: Singlet-E 1.9940 eV 621.77 nm f=0.0067 <S**2>=0.000
243 ->252 -0.14147
246 ->252 -0.19284
247 ->252 0.64832

Excited State 30: Singlet-E 1.9940 eV 621.77 nm f=0.0067 <S**2>=0.000
242 ->252 -0.14147
246 ->252 0.64832
247 ->252 0.19283

Excited State 31: Singlet-B 1.9955 eV 621.30 nm f=0.0035 <S**2>=0.000
245 ->252 0.64815
249 ->252 -0.25717

Excited State 32: Singlet-A 2.0298 eV 610.82 nm f=0.0000 <S**2>=0.000
234 ->250 -0.17479
235 ->251 -0.17487
244 ->252 0.52538
248 ->252 0.39284

Excited State 33: Singlet-E 2.0474 eV 605.57 nm f=0.0666 <S**2>=0.000
236 ->250 0.43990
237 ->250 0.22339
242 ->252 -0.38982
243 ->252 0.27934

Excited State 34: Singlet-E 2.0474 eV 605.57 nm f=0.0666 <S**2>=0.000
236 ->251 0.43990
237 ->251 -0.22340
242 ->252 -0.27933
243 ->252 -0.38981

Excited State 35: Singlet-E 2.0801 eV 596.06 nm f=0.0773 <S**2>=0.000
236 ->250 0.11203
236 ->251 0.49609
242 ->252 0.29322
243 ->252 0.32963
246 ->252 0.12072

Excited State 36: Singlet-E 2.0801 eV 596.06 nm f=0.0773 <S**2>=0.000
236 ->250 0.49609
236 ->251 -0.11203

242 ->252 0.32963
243 ->252 -0.29322
247 ->252 -0.12072

Excited state symmetry could not be determined.
Excited State 37: Singlet-?Sym 2.1140 eV 586.49 nm f=0.0049 <S**2>=0.000
234 ->250 -0.10390
234 ->251 0.48636
235 ->250 0.48439
235 ->251 0.10431

Excited state symmetry could not be determined.
Excited State 38: Singlet-?Sym 2.1176 eV 585.50 nm f=0.0000 <S**2>=0.000
234 ->250 -0.14445
234 ->251 -0.47021
235 ->250 0.47226
235 ->251 -0.14442

Excited State 39: Singlet-E 2.1431 eV 578.53 nm f=0.0002 <S**2>=0.000
233 ->250 0.43098
233 ->251 0.55874

Excited State 40: Singlet-E 2.1431 eV 578.53 nm f=0.0002 <S**2>=0.000
233 ->250 0.55874
233 ->251 -0.43098

Excited state symmetry could not be determined.
Excited State 41: Singlet-?Sym 2.1491 eV 576.92 nm f=0.0223 <S**2>=0.000
234 ->250 0.46753
234 ->251 0.11202
235 ->250 0.11187
235 ->251 -0.46673
249 ->252 -0.16339

Excited state symmetry could not be determined.
Excited State 42: Singlet-?Sym 2.1919 eV 565.63 nm f=0.0000 <S**2>=0.000
234 ->250 0.43406
234 ->251 -0.15915
235 ->250 0.15919
235 ->251 0.43479
244 ->252 0.13840
248 ->252 0.16721

Excited State 43: Singlet-B 2.4005 eV 516.50 nm f=0.0036 <S**2>=0.000
241 ->252 0.70001

Excited State 44: Singlet-E 2.4067 eV 515.15 nm f=0.0068 <S**2>=0.000
239 ->252 0.69783

Excited State 45: Singlet-E 2.4067 eV 515.15 nm f=0.0068 <S**2>=0.000
238 ->252 0.69783

Excited State 46: Singlet-A 2.4087 eV 514.74 nm f=0.0000 <S**2>=0.000
240 ->252 0.69955

Excited State 47: Singlet-E 2.5112 eV 493.73 nm f=0.0344 <S**2>=0.000
225 ->251 -0.10810
229 ->250 -0.31082
232 ->251 0.58653

Excited State 48: Singlet-E 2.5112 eV 493.73 nm f=0.0344 <S**2>=0.000
225 ->250 -0.10810
229 ->251 0.31083
232 ->250 0.58653

Excited state symmetry could not be determined.
Excited State 49: Singlet-?Sym 2.5132 eV 493.34 nm f=0.0000 <S**2>=0.000
230 ->250 0.31684
230 ->251 -0.38674
231 ->250 0.38675
231 ->251 0.31679

Excited state symmetry could not be determined.
Excited State 50: Singlet-?Sym 2.5224 eV 491.54 nm f=0.0001 <S**2>=0.000
230 ->250 0.45202
230 ->251 -0.21331
231 ->250 -0.21337
231 ->251 -0.45201

Excited State 51: Singlet-A 2.5614 eV 484.05 nm f=0.0000 <S**2>=0.000
244 ->256 -0.14169
245 ->257 -0.17883
246 ->258 -0.15501
247 ->259 -0.15518
248 ->256 0.10642
249 ->253 0.58894

Excited State 52: Singlet-E 2.5745 eV 481.58 nm f=0.0008 <S**2>=0.000
242 ->253 -0.10455
243 ->256 -0.12281

244 ->258 0.12364
245 ->255 0.19668
245 ->258 0.12416
246 ->256 0.11596
246 ->257 0.16651
247 ->253 0.26825
248 ->258 -0.10984
249 ->254 0.42255
249 ->259 0.17843

Excited State 53: Singlet-E 2.5745 eV 481.58 nm f=0.0008 <S**2>=0.000
242 ->256 0.12283
243 ->253 0.10455
244 ->259 0.12364
245 ->254 -0.19668
245 ->259 -0.12416
246 ->253 0.26824
247 ->256 0.11592
247 ->257 -0.16654
248 ->259 -0.10985
249 ->255 0.42256
249 ->258 0.17842

Excited State 54: Singlet-B 2.5788 eV 480.78 nm f=0.0000 <S**2>=0.000
242 ->258 0.14775
243 ->259 -0.14932
244 ->253 0.23956
244 ->257 -0.13704
246 ->254 -0.23734
247 ->255 -0.23976
248 ->253 -0.29901
248 ->257 -0.13683
249 ->256 0.36916

Excited State 55: Singlet-A 2.5796 eV 480.63 nm f=0.0000 <S**2>=0.000
242 ->258 0.12832
243 ->259 0.12652
244 ->256 -0.11589
245 ->253 0.38924
246 ->254 -0.20511
247 ->255 0.20226
248 ->256 -0.16475
249 ->257 0.37253

Excited State 56: Singlet-E 2.5812 eV 480.33 nm f=0.0002 <S**2>=0.000

242 ->253 0.15851
243 ->253 -0.11077
243 ->257 0.12614
244 ->255 -0.19568
245 ->255 0.15443
245 ->258 -0.15853
246 ->256 -0.14994
247 ->253 0.23893
248 ->254 0.16796
248 ->255 0.11019
248 ->259 0.12113
249 ->254 -0.23572
249 ->259 0.31576

Excited State 57: Singlet-E 2.5812 eV 480.33 nm f=0.0002 <S**2>=0.000
242 ->253 -0.11077
242 ->257 0.12612
243 ->253 -0.15851
244 ->254 -0.19570
245 ->254 -0.15443
245 ->259 0.15853
246 ->253 0.23893
247 ->256 -0.14992
248 ->254 0.11018
248 ->255 -0.16795
248 ->258 -0.12113
249 ->255 -0.23571
249 ->258 0.31576

Excited State 58: Singlet-B 2.5924 eV 478.26 nm f=0.0000 <S**2>=0.000
242 ->254 0.17408
243 ->255 0.17392
244 ->253 0.31134
244 ->257 0.14565
245 ->256 0.21197
246 ->255 0.11960
246 ->258 0.18787
247 ->254 -0.11957
247 ->259 -0.18767
248 ->253 0.34302
248 ->257 -0.15493

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 2.6054 eV 475.88 nm f=0.0000 <S**2>=0.000
226 ->250 -0.14700

226 ->251 0.10143
227 ->250 -0.10293
227 ->251 -0.14827
230 ->250 0.36053
230 ->251 0.29786
231 ->250 -0.29372
231 ->251 0.35865

Excited state symmetry could not be determined.
Excited State 60: Singlet-?Sym 2.6058 eV 475.80 nm f=0.0011 <S**2>=0.000
226 ->250 0.11534
226 ->251 -0.15258
227 ->250 -0.15155
227 ->251 -0.11389
230 ->250 0.19143
230 ->251 0.41372
231 ->250 0.41661
231 ->251 -0.19499

Excited State 61: Singlet-E 2.6321 eV 471.05 nm f=0.0050 <S**2>=0.000
242 ->253 0.30577
244 ->254 0.15356
246 ->253 0.19113
247 ->253 -0.24707
248 ->254 0.21719
249 ->254 0.41992

Excited State 62: Singlet-E 2.6321 eV 471.05 nm f=0.0050 <S**2>=0.000
243 ->253 -0.30577
244 ->255 -0.15355
246 ->253 -0.24707
247 ->253 -0.19114
248 ->255 -0.21717
249 ->255 0.41992

Excited State 63: Singlet-A 2.6405 eV 469.55 nm f=0.0000 <S**2>=0.000
242 ->254 0.18109
243 ->255 -0.18120
245 ->253 0.34230
245 ->257 0.10816
246 ->254 0.30014
247 ->255 -0.30043
249 ->253 0.24286

Excited State 64: Singlet-B 2.6438 eV 468.96 nm f=0.0003 <S**2>=0.000

244 ->253 -0.21896
246 ->254 -0.32147
247 ->255 -0.32109
248 ->253 0.45762
249 ->256 0.10412

Excited State 65: Singlet-E 2.6460 eV 468.58 nm f=0.0002 <S**2>=0.000
242 ->253 0.11526
245 ->255 -0.23483
246 ->253 -0.13189
247 ->253 0.41871
248 ->254 0.25626
248 ->255 -0.33668
249 ->254 0.10212
249 ->259 -0.14409

Excited State 66: Singlet-E 2.6460 eV 468.58 nm f=0.0002 <S**2>=0.000
243 ->253 -0.11527
245 ->254 0.23484
246 ->253 0.41871
247 ->253 0.13188
248 ->254 -0.33666
248 ->255 -0.25626
249 ->255 0.10213
249 ->258 -0.14410

Excited State 67: Singlet-E 2.6471 eV 468.37 nm f=0.0055 <S**2>=0.000
225 ->250 0.11306
228 ->250 0.67955

Excited State 68: Singlet-E 2.6471 eV 468.37 nm f=0.0055 <S**2>=0.000
225 ->251 -0.11305
228 ->251 0.67955

Excited State 69: Singlet-A 2.6516 eV 467.59 nm f=0.0000 <S**2>=0.000
226 ->250 -0.10709
226 ->251 -0.22335
227 ->250 0.22336
227 ->251 -0.10704
242 ->254 -0.24024
243 ->255 0.24029
245 ->253 0.35938
246 ->254 0.11659
246 ->255 0.12954
247 ->254 0.12954

247 ->255 -0.11671
249 ->253 -0.14205
249 ->257 -0.12807

Excited state symmetry could not be determined.
Excited State 70: Singlet-?Sym 2.6547 eV 467.03 nm f=0.0000 <S**2>=0.000
226 ->250 -0.16778
226 ->251 -0.39259
227 ->250 0.39328
227 ->251 -0.16835
242 ->254 0.14231
243 ->255 -0.14234
245 ->253 -0.16070
246 ->255 -0.12883
247 ->254 -0.12885
249 ->253 0.10887

Excited state symmetry could not be determined.
Excited State 71: Singlet-?Sym 2.6559 eV 466.82 nm f=0.0004 <S**2>=0.000
226 ->250 0.31297
226 ->251 0.38149
227 ->250 0.38087
227 ->251 -0.31256

Excited State 72: Singlet-B 2.6594 eV 466.21 nm f=0.0004 <S**2>=0.000
242 ->254 -0.18106
243 ->255 -0.18093
244 ->253 0.39612
246 ->255 -0.35702
247 ->254 0.35724
248 ->253 0.10567

Excited State 73: Singlet-E 2.6609 eV 465.95 nm f=0.0040 <S**2>=0.000
225 ->250 0.18883
225 ->251 0.19731
229 ->251 0.12410
242 ->253 0.35403
243 ->253 -0.14365
245 ->254 -0.28595
245 ->255 -0.18452
248 ->254 -0.30708
249 ->259 0.11051

Excited State 74: Singlet-E 2.6609 eV 465.95 nm f=0.0040 <S**2>=0.000
225 ->250 -0.19732

225 ->251 0.18883
229 ->250 -0.12411
242 ->253 0.14365
243 ->253 0.35403
245 ->254 -0.18453
245 ->255 0.28595
248 ->255 -0.30707
249 ->258 -0.11054

Excited State 75: Singlet-E 2.6633 eV 465.52 nm f=0.0089 <S**2>=0.000
225 ->250 0.46798
225 ->251 0.28730
229 ->250 0.11801
229 ->251 0.22084
232 ->251 0.10510
242 ->253 -0.16225
243 ->253 0.12720
245 ->254 0.13743
245 ->255 0.11967
248 ->254 0.14769

Excited State 76: Singlet-E 2.6633 eV 465.52 nm f=0.0089 <S**2>=0.000
225 ->250 -0.28730
225 ->251 0.46798
229 ->250 -0.22084
229 ->251 0.11801
232 ->250 -0.10510
242 ->253 -0.12719
243 ->253 -0.16226
245 ->254 0.11967
245 ->255 -0.13743
248 ->255 0.14769

Excited State 77: Singlet-B 2.6652 eV 465.20 nm f=0.0001 <S**2>=0.000
242 ->254 0.10383
242 ->258 -0.13738
243 ->255 0.10403
243 ->259 0.13734
244 ->253 -0.16678
244 ->257 0.15742
246 ->254 0.10619
246 ->255 -0.16009
247 ->254 0.15932
247 ->255 0.10611
248 ->257 0.20665

249 ->256 0.47962

Excited state symmetry could not be determined.
Excited State 78: Singlet-?Sym 2.6667 eV 464.93 nm f=0.0000 <S**2>=0.000
242 ->254 0.20480
243 ->255 -0.20453
246 ->255 0.42124
247 ->254 0.42136
249 ->257 -0.15683

Excited State 79: Singlet-A 2.6684 eV 464.64 nm f=0.0000 <S**2>=0.000
242 ->258 -0.13552
243 ->259 -0.13556
244 ->256 0.14549
246 ->255 0.15138
247 ->254 0.15170
248 ->256 0.29941
249 ->257 0.47811

Excited State 80: Singlet-E 2.6685 eV 464.63 nm f=0.0001 <S**2>=0.000
242 ->256 -0.12170
242 ->257 -0.12307
244 ->255 0.25720
244 ->258 0.10374
245 ->254 0.19241
245 ->255 0.19210
246 ->257 -0.10280
248 ->258 0.24601
249 ->258 0.44967

Excited State 81: Singlet-E 2.6685 eV 464.63 nm f=0.0001 <S**2>=0.000
243 ->256 0.12165
243 ->257 -0.12308
244 ->254 -0.25731
244 ->259 -0.10371
245 ->254 0.19215
245 ->255 -0.19239
247 ->257 -0.10283
248 ->259 -0.24598
249 ->259 0.44963

Excited state symmetry could not be determined.
Excited State 82: Singlet-?Sym 2.6707 eV 464.24 nm f=0.0004 <S**2>=0.000
242 ->254 0.27845
243 ->255 0.27840

244 ->253 -0.20396
246 ->255 -0.27731
246 ->258 0.10687
247 ->254 0.27715
247 ->259 -0.10674
248 ->257 -0.20432
249 ->256 -0.19560

Excited State 83: Singlet-E 2.6719 eV 464.02 nm f=0.0000 <S**2>=0.000
242 ->253 -0.25663
244 ->254 0.49172
244 ->259 -0.12049
245 ->254 -0.24790
248 ->259 -0.12274
249 ->259 0.20610

Excited State 84: Singlet-E 2.6719 eV 464.02 nm f=0.0000 <S**2>=0.000
243 ->253 -0.25660
244 ->255 0.49179
244 ->258 -0.12047
245 ->255 0.24794
248 ->258 -0.12269
249 ->258 -0.20600

Excited state symmetry could not be determined.
Excited State 85: Singlet-?Sym 2.6740 eV 463.67 nm f=0.0002 <S**2>=0.000
226 ->250 0.36809
226 ->251 -0.27052
227 ->250 -0.26741
227 ->251 -0.36036
230 ->251 -0.15693
231 ->250 -0.15882

Excited state symmetry could not be determined.
Excited State 86: Singlet-?Sym 2.6746 eV 463.55 nm f=0.0000 <S**2>=0.000
226 ->250 0.41912
226 ->251 -0.16912
227 ->250 0.17391
227 ->251 0.42574
230 ->250 0.13368
230 ->251 0.10840
231 ->250 -0.10556
231 ->251 0.13230
249 ->257 -0.10338

Excited state symmetry could not be determined.
Excited State 87: Singlet-?Sym 2.6917 eV 460.62 nm f=0.0000 <S**2>=0.000
242 ->255 0.47285
243 ->254 0.47626
248 ->256 0.14692

Excited state symmetry could not be determined.
Excited State 88: Singlet-?Sym 2.6918 eV 460.60 nm f=0.0000 <S**2>=0.000
242 ->255 0.46988
243 ->254 -0.46643
248 ->257 0.18356

Excited State 89: Singlet-E 2.6997 eV 459.25 nm f=0.0000 <S**2>=0.000
246 ->256 -0.21680
246 ->257 -0.18334
247 ->256 0.41012
248 ->258 -0.39726
248 ->259 0.24345

Excited State 90: Singlet-E 2.6997 eV 459.25 nm f=0.0000 <S**2>=0.000
246 ->256 0.41005
247 ->256 0.21679
247 ->257 -0.18342
248 ->258 0.24347
248 ->259 0.39727

Excited State 91: Singlet-A 2.7002 eV 459.16 nm f=0.0000 <S**2>=0.000
244 ->256 -0.17086
246 ->258 0.29068
246 ->259 0.16312
247 ->258 -0.16323
247 ->259 0.29065
248 ->256 0.45899

Excited State 92: Singlet-B 2.7010 eV 459.03 nm f=0.0000 <S**2>=0.000
244 ->257 -0.11438
246 ->258 0.27150
246 ->259 -0.21939
247 ->258 -0.21943
247 ->259 -0.27159
248 ->257 0.46348

Excited State 93: Singlet-E 2.7029 eV 458.71 nm f=0.0000 <S**2>=0.000
245 ->258 -0.21401
246 ->256 0.17609

246 ->257 0.15060
247 ->256 0.28501
247 ->257 0.51382
248 ->259 -0.16434

Excited State 94: Singlet-E 2.7029 eV 458.71 nm f=0.0000 <S**2>=0.000
245 ->259 0.21405
246 ->256 -0.28495
246 ->257 0.51389
247 ->256 0.17603
247 ->257 -0.15061
248 ->258 0.16430

Excited State 95: Singlet-B 2.7029 eV 458.70 nm f=0.0000 <S**2>=0.000
245 ->256 0.46073
246 ->258 -0.22184
246 ->259 -0.29920
247 ->258 -0.29951
247 ->259 0.22163

Excited state symmetry could not be determined.
Excited State 96: Singlet-?Sym 2.7038 eV 458.56 nm f=0.0000 <S**2>=0.000
245 ->257 0.17925
246 ->258 -0.14936
246 ->259 0.44712
247 ->258 -0.44691
247 ->259 -0.14946

Excited State 97: Singlet-A 2.7060 eV 458.18 nm f=0.0000 <S**2>=0.000
244 ->256 -0.28653
245 ->257 0.57216
246 ->258 -0.12426
246 ->259 -0.10841
247 ->258 0.10973
247 ->259 -0.12433
248 ->256 0.12920

Excited State 98: Singlet-B 2.7063 eV 458.14 nm f=0.0000 <S**2>=0.000
242 ->258 0.11507
243 ->259 -0.11547
244 ->257 -0.34199
245 ->256 0.37888
246 ->259 0.29852
247 ->258 0.29796
248 ->257 0.17083

Excited State 99: Singlet-E 2.7068 eV 458.05 nm f=0.0000 <S**2>=0.000
242 ->256 0.11444
242 ->257 0.10805
244 ->258 -0.27641
245 ->258 0.55508
246 ->257 -0.10300
247 ->256 0.14610
247 ->257 0.10797
248 ->258 0.16876

Excited State 100: Singlet-E 2.7068 eV 458.05 nm f=0.0000 <S**2>=0.000
243 ->256 -0.11443
243 ->257 0.10810
244 ->259 0.27645
245 ->259 0.55505
246 ->256 0.14609
246 ->257 -0.10803
247 ->257 -0.10299
248 ->259 -0.16875

Excited State 101: Singlet-A 2.7187 eV 456.04 nm f=0.0000 <S**2>=0.000
242 ->258 0.32300
243 ->259 0.32300
244 ->256 0.48018
248 ->256 0.15456

Excited State 102: Singlet-E 2.7197 eV 455.88 nm f=0.0000 <S**2>=0.000
242 ->256 0.34942
242 ->257 0.27845
244 ->258 0.50173
248 ->258 0.12435

Excited State 103: Singlet-E 2.7197 eV 455.88 nm f=0.0000 <S**2>=0.000
243 ->256 0.34935
243 ->257 -0.27853
244 ->259 0.50174
248 ->259 0.12435

Excited State 104: Singlet-B 2.7209 eV 455.67 nm f=0.0000 <S**2>=0.000
242 ->258 0.34045
243 ->259 -0.34047
244 ->257 0.47094
248 ->257 0.13579

Excited State 105: Singlet-E 2.7295 eV 454.24 nm f=0.0001 <S**2>=0.000
243 ->256 0.46367
243 ->257 0.51999

Excited State 106: Singlet-E 2.7295 eV 454.24 nm f=0.0001 <S**2>=0.000
242 ->256 -0.46355
242 ->257 0.52010

Excited state symmetry could not be determined.
Excited State 107: Singlet-?Sym 2.7305 eV 454.06 nm f=0.0000 <S**2>=0.000
242 ->259 -0.48095
243 ->258 0.48209

Excited state symmetry could not be determined.
Excited State 108: Singlet-?Sym 2.7311 eV 453.97 nm f=0.0000 <S**2>=0.000
242 ->259 0.49399
243 ->258 0.49286

Excited State 109: Singlet-B 2.7902 eV 444.35 nm f=0.0002 <S**2>=0.000
242 ->254 -0.14151
243 ->255 -0.14156
249 ->260 0.63286

Excited State 110: Singlet-A 2.8204 eV 439.60 nm f=0.0000 <S**2>=0.000
242 ->258 0.14624
243 ->259 0.14631
244 ->256 -0.10535
244 ->260 -0.22643
245 ->253 -0.12142
246 ->254 0.16058
247 ->255 -0.16074
248 ->260 0.53496

Excited State 111: Singlet-E 2.8211 eV 439.48 nm f=0.0016 <S**2>=0.000
243 ->256 -0.13534
243 ->257 0.14636
244 ->259 0.11481
245 ->255 -0.15709
247 ->253 -0.13774
247 ->260 0.56704
248 ->255 -0.13047

Excited State 112: Singlet-E 2.8211 eV 439.48 nm f=0.0016 <S**2>=0.000
242 ->256 -0.13537
242 ->257 -0.14632

244 ->258 0.11482
245 ->254 -0.15709
246 ->253 0.13774
246 ->260 0.56704
248 ->254 0.13046

Excited State 113: Singlet-B 2.8223 eV 439.29 nm f=0.0000 <S**2>=0.000
242 ->258 -0.12761
243 ->259 0.12748
244 ->253 0.12613
245 ->260 0.56890
246 ->254 -0.14411
247 ->255 -0.14397

Excited State 114: Singlet-A 2.8361 eV 437.16 nm f=0.0000 <S**2>=0.000
242 ->254 0.16896
243 ->255 -0.16893
244 ->260 0.50768
246 ->258 -0.10408
247 ->259 -0.10407
248 ->256 0.10892
248 ->260 0.24512

Excited State 115: Singlet-E 2.8424 eV 436.20 nm f=0.0249 <S**2>=0.000
239 ->253 0.12262
240 ->255 0.10453
241 ->255 0.12378
243 ->253 -0.16780
243 ->260 0.51246
244 ->255 -0.15519
245 ->259 -0.12617
247 ->256 0.12689
247 ->257 -0.13850
248 ->259 -0.11375
249 ->255 -0.11315

Excited State 116: Singlet-E 2.8424 eV 436.20 nm f=0.0249 <S**2>=0.000
238 ->253 0.12262
240 ->254 -0.10454
241 ->254 0.12378
242 ->253 0.16780
242 ->260 0.51246
244 ->254 0.15519
245 ->258 0.12617
246 ->256 0.12693

246 ->257 0.13847
248 ->258 -0.11374
249 ->254 -0.11315

Excited State 117: Singlet-B 2.9253 eV 423.83 nm f=0.0038 <S**2>=0.000
237 ->252 0.14761
238 ->254 -0.28009
239 ->255 0.28053
240 ->253 0.36639
241 ->260 0.12147
242 ->254 -0.12906
243 ->255 -0.12928
245 ->256 0.13125
246 ->258 0.13560
247 ->259 -0.13582
249 ->260 -0.18759

Excited State 118: Singlet-A 2.9302 eV 423.13 nm f=0.0000 <S**2>=0.000
238 ->254 0.26548
239 ->255 0.26509
240 ->260 0.10590
241 ->253 0.39360
244 ->260 -0.21970
245 ->257 -0.11534
246 ->258 -0.10203
247 ->259 -0.10190
248 ->260 -0.24048

Excited State 119: Singlet-E 2.9332 eV 422.70 nm f=0.0001 <S**2>=0.000
238 ->253 0.12167
239 ->256 0.23986
239 ->257 -0.23927
240 ->254 -0.16253
240 ->259 -0.21938
241 ->259 -0.25181
243 ->256 0.11414
243 ->257 -0.13537
244 ->259 -0.10623
247 ->260 0.33648

Excited State 120: Singlet-E 2.9332 eV 422.70 nm f=0.0001 <S**2>=0.000
238 ->256 -0.23991
238 ->257 -0.23920
239 ->253 -0.12170
240 ->255 -0.16255

240 ->258 -0.21938
241 ->258 0.25179
242 ->256 0.11417
242 ->257 0.13534
244 ->258 -0.10623
246 ->260 0.33647

Excited State 121: Singlet-B 2.9348 eV 422.46 nm f=0.0000 <S**2>=0.000
238 ->258 -0.25493
239 ->259 -0.25108
240 ->257 -0.26083
241 ->256 0.26128
242 ->258 0.12824
243 ->259 -0.12625
244 ->257 -0.10312
245 ->260 0.34237
249 ->256 0.10589

Excited State 122: Singlet-A 2.9357 eV 422.33 nm f=0.0000 <S**2>=0.000
238 ->258 -0.25077
239 ->259 0.25461
240 ->256 -0.26507
241 ->257 0.26129
242 ->258 0.13217
243 ->259 0.13417
244 ->260 0.29342
247 ->255 -0.10053
248 ->260 -0.20420
249 ->257 0.10695

Excited State 123: Singlet-E 2.9366 eV 422.20 nm f=0.0032 <S**2>=0.000
239 ->253 -0.31062
240 ->255 -0.22298
240 ->258 0.13010
241 ->255 -0.29476
243 ->260 0.38435
247 ->257 0.10013

Excited State 124: Singlet-E 2.9366 eV 422.20 nm f=0.0032 <S**2>=0.000
238 ->253 -0.31063
240 ->254 0.22302
240 ->259 -0.13008
241 ->254 -0.29475
242 ->260 0.38435
246 ->257 -0.10011

Excited State 125: Singlet-B 2.9753 eV 416.71 nm f=0.0589 <S**2>=0.000
237 ->252 0.66218
240 ->253 -0.10439

Excited State 126: Singlet-E 3.0331 eV 408.77 nm f=0.0334 <S**2>=0.000
224 ->250 0.68497
224 ->251 0.10452

Excited State 127: Singlet-E 3.0331 eV 408.77 nm f=0.0334 <S**2>=0.000
224 ->250 -0.10452
224 ->251 0.68497

Excited state symmetry could not be determined.
Excited State 128: Singlet-?Sym 3.0424 eV 407.52 nm f=0.0001 <S**2>=0.000
222 ->251 0.48847
223 ->250 0.48924

Excited state symmetry could not be determined.
Excited State 129: Singlet-?Sym 3.0450 eV 407.17 nm f=0.0000 <S**2>=0.000
222 ->250 0.23674
222 ->251 0.43292
223 ->250 -0.43211
223 ->251 0.23708

Excited State 130: Singlet-E 3.0536 eV 406.02 nm f=0.1433 <S**2>=0.000
221 ->250 0.39849
221 ->251 -0.31476
225 ->251 -0.12526
229 ->250 -0.14656
229 ->251 0.18269
234 ->252 0.12636
238 ->253 0.18454
239 ->253 -0.17958
241 ->254 -0.14957
241 ->255 0.16060

Excited State 131: Singlet-E 3.0536 eV 406.02 nm f=0.1433 <S**2>=0.000
221 ->250 0.31476
221 ->251 0.39849
225 ->250 0.12526
229 ->250 -0.18269
229 ->251 -0.14656
235 ->252 -0.12636
238 ->253 -0.17958

239 ->253 -0.18456
241 ->254 0.16060
241 ->255 0.14958

Excited state symmetry could not be determined.
Excited State 132: Singlet-?Sym 3.0550 eV 405.84 nm f=0.0000 <S**2>=0.000
222 ->250 0.41136
222 ->251 -0.24456
223 ->250 0.24415
223 ->251 0.41054
241 ->253 -0.15426

Excited State 133: Singlet-A 3.0582 eV 405.41 nm f=0.0000 <S**2>=0.000
222 ->250 0.13595
223 ->251 0.13549
238 ->254 -0.32518
239 ->255 -0.32523
241 ->253 0.49601

Excited state symmetry could not be determined.
Excited State 134: Singlet-?Sym 3.0591 eV 405.29 nm f=0.0021 <S**2>=0.000
222 ->250 -0.47886
223 ->251 0.47945
237 ->252 -0.10183

Excited State 135: Singlet-E 3.0610 eV 405.05 nm f=0.0219 <S**2>=0.000
221 ->250 0.28512
229 ->250 -0.10038
239 ->253 0.49154
240 ->255 -0.22805
241 ->255 -0.30950

Excited State 136: Singlet-E 3.0610 eV 405.05 nm f=0.0219 <S**2>=0.000
221 ->251 0.28511
229 ->251 -0.10037
238 ->253 0.49155
240 ->254 0.22807
241 ->254 -0.30950

Excited State 137: Singlet-B 3.0619 eV 404.92 nm f=0.0004 <S**2>=0.000
238 ->254 0.31733
239 ->255 -0.31731
240 ->253 0.53761

Excited State 138: Singlet-E 3.0762 eV 403.05 nm f=0.0004 <S**2>=0.000

221 ->251 -0.11203
240 ->254 0.53857
241 ->254 0.41965

Excited State 139: Singlet-E 3.0762 eV 403.05 nm f=0.0004 <S**2>=0.000
221 ->250 0.11203
240 ->255 0.53860
241 ->255 -0.41962

Excited state symmetry could not be determined.
Excited State 140: Singlet-?Sym 3.0830 eV 402.15 nm f=0.0000 <S**2>=0.000
238 ->255 0.48938
239 ->254 0.49494

Excited state symmetry could not be determined.
Excited State 141: Singlet-?Sym 3.0831 eV 402.14 nm f=0.0000 <S**2>=0.000
238 ->255 0.49521
239 ->254 -0.48965

Excited State 142: Singlet-B 3.1100 eV 398.66 nm f=0.0000 <S**2>=0.000
238 ->258 0.16828
239 ->259 0.16820
240 ->257 0.25321
241 ->256 0.61379

Excited State 143: Singlet-A 3.1114 eV 398.48 nm f=0.0000 <S**2>=0.000
238 ->258 0.13300
239 ->259 -0.13315
240 ->256 0.31010
241 ->257 0.60626

Excited State 144: Singlet-E 3.1117 eV 398.45 nm f=0.0010 <S**2>=0.000
238 ->256 0.19302
238 ->257 0.14742
240 ->258 0.22219
241 ->258 0.61506

Excited State 145: Singlet-E 3.1117 eV 398.45 nm f=0.0010 <S**2>=0.000
239 ->256 0.19302
239 ->257 -0.14748
240 ->259 -0.22219
241 ->259 0.61504

Excited State 146: Singlet-A 3.1190 eV 397.51 nm f=0.0000 <S**2>=0.000
238 ->258 -0.32292

239 ->259 0.32287
240 ->256 0.51921
241 ->257 -0.12242

Excited State 147: Singlet-E 3.1196 eV 397.44 nm f=0.0010 <S**2>=0.000
239 ->256 0.49128
240 ->259 0.49857

Excited State 148: Singlet-E 3.1196 eV 397.44 nm f=0.0010 <S**2>=0.000
238 ->256 -0.49119
240 ->258 0.49865

Excited State 149: Singlet-B 3.1204 eV 397.34 nm f=0.0000 <S**2>=0.000
238 ->258 -0.30604
239 ->259 -0.30607
240 ->257 0.54922

Excited State 150: Singlet-E 3.1212 eV 397.23 nm f=0.0008 <S**2>=0.000
239 ->256 0.29134
239 ->257 0.58488
240 ->259 -0.26043

Table S2: Vertical Excitation energies of TAP^{FcCN}Mg using BPW91 PCM-TDDFT
Excited State 1: Singlet-E 0.6418 eV 1931.78 nm f=0.0004 <S**2>=0.000
269 ->275 -0.33809
272 ->274 0.37852
272 ->275 -0.44413
273 ->274 0.20225
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3459.46916212
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-E 0.6418 eV 1931.78 nm f=0.0004 <S**2>=0.000
269 ->274 -0.33808
272 ->274 0.44413
272 ->275 0.37852
273 ->275 0.20225

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 0.6440 eV 1925.15 nm f=0.0000 <S**2>=0.000
270 ->274 -0.49468
271 ->275 0.49466

Excited State 4: Singlet-E 0.6481 eV 1913.09 nm f=0.0002 <S**2>=0.000
269 ->274 0.19939
269 ->275 0.57781
272 ->274 0.27669
272 ->275 -0.21498

Excited State 5: Singlet-E 0.6481 eV 1913.09 nm f=0.0002 <S**2>=0.000
269 ->274 -0.57781
269 ->275 0.19939
272 ->274 -0.21497
272 ->275 -0.27669

Excited state symmetry could not be determined.
Excited State 6: Singlet-?Sym 0.6484 eV 1912.20 nm f=0.0000 <S**2>=0.000
270 ->275 0.49187
271 ->274 0.49615

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 0.6487 eV 1911.29 nm f=0.0000 <S**2>=0.000
270 ->275 0.50124
271 ->274 -0.49702

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 0.6498 eV 1908.05 nm f=0.0002 <S**2>=0.000
270 ->274 0.48996
271 ->275 0.49005

Excited State 9: Singlet-E 0.6718 eV 1845.59 nm f=0.0085 <S**2>=0.000
268 ->275 0.48181
272 ->275 -0.15913
273 ->274 -0.23940
273 ->275 0.41285

Excited State 10: Singlet-E 0.6718 eV 1845.59 nm f=0.0085 <S**2>=0.000
268 ->274 0.48181
272 ->274 0.15913
273 ->274 -0.41285
273 ->275 -0.23940

Excited state symmetry could not be determined.
Excited State 11: Singlet-?Sym 0.7199 eV 1722.20 nm f=0.0000 <S**2>=0.000
266 ->274 0.47813
266 ->275 0.14552
267 ->274 0.14553

267 ->275 -0.47812

Excited state symmetry could not be determined.
Excited State 12: Singlet-?Sym 0.7333 eV 1690.66 nm f=0.0000 <S**2>=0.000
266 ->274 0.46121
266 ->275 0.19138
267 ->274 -0.19139
267 ->275 0.46122

Excited state symmetry could not be determined.
Excited State 13: Singlet-?Sym 0.8937 eV 1387.31 nm f=0.0177 <S**2>=0.000
262 ->274 -0.10780
263 ->275 -0.10782
266 ->274 -0.17938
266 ->275 0.43702
267 ->274 -0.43699
267 ->275 -0.17937
273 ->276 0.11227

Excited State 14: Singlet-E 0.9015 eV 1375.26 nm f=0.1550 <S**2>=0.000
264 ->275 0.13493
265 ->275 -0.17857
268 ->274 -0.23572
268 ->275 0.42357
273 ->275 -0.43902

Excited State 15: Singlet-E 0.9015 eV 1375.26 nm f=0.1550 <S**2>=0.000
264 ->274 0.13493
265 ->274 0.17857
268 ->274 0.42357
268 ->275 0.23572
273 ->274 0.43902

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 0.9381 eV 1321.65 nm f=0.0000 <S**2>=0.000
262 ->274 0.11768
262 ->275 0.14736
263 ->274 0.14737
263 ->275 -0.11767
266 ->274 -0.13498
266 ->275 0.43826
267 ->274 0.43829
267 ->275 0.13499
268 ->276 -0.10321

Excited State 17: Singlet-E 1.0345 eV 1198.54 nm f=0.0049 <S**2>=0.000
264 ->274 0.10411
264 ->275 0.46239
265 ->274 -0.36899
265 ->275 0.36821

Excited State 18: Singlet-E 1.0345 eV 1198.54 nm f=0.0049 <S**2>=0.000
264 ->274 0.46239
264 ->275 -0.10411
265 ->274 -0.36821
265 ->275 -0.36899

Excited state symmetry could not be determined.
Excited State 19: Singlet-?Sym 1.0456 eV 1185.74 nm f=0.0000 <S**2>=0.000
262 ->274 0.40008
262 ->275 -0.29972
263 ->274 -0.29973
263 ->275 -0.40007

Excited state symmetry could not be determined.
Excited State 20: Singlet-?Sym 1.0482 eV 1182.86 nm f=0.0000 <S**2>=0.000
262 ->274 0.16256
262 ->275 0.47255
263 ->274 -0.47254
263 ->275 0.16257

Excited State 21: Singlet-E 1.1186 eV 1108.38 nm f=0.0961 <S**2>=0.000
264 ->274 -0.39938
264 ->275 0.30410
265 ->274 -0.14548
265 ->275 -0.41206
268 ->274 0.11587
273 ->275 0.16093

Excited State 22: Singlet-E 1.1186 eV 1108.38 nm f=0.0961 <S**2>=0.000
264 ->274 0.30410
264 ->275 0.39938
265 ->274 0.41206
265 ->275 -0.14548
268 ->275 -0.11587
273 ->274 -0.16093

Excited state symmetry could not be determined.
Excited State 23: Singlet-?Sym 1.1194 eV 1107.58 nm f=0.0082 <S**2>=0.000
262 ->274 0.45739

262 ->275 -0.15599
263 ->274 0.15610
263 ->275 0.45731

Excited state symmetry could not be determined.
Excited State 24: Singlet-?Sym 1.1446 eV 1083.26 nm f=0.0000 <S**2>=0.000
262 ->274 0.27323
262 ->275 0.36938
263 ->274 0.36933
263 ->275 -0.27336
266 ->275 -0.16945
267 ->274 -0.16942
268 ->276 0.10916

Excited State 25: Singlet-B 1.5146 eV 818.57 nm f=0.0001 <S**2>=0.000
272 ->276 0.69771
273 ->276 0.10957

Excited State 26: Singlet-E 1.5171 eV 817.25 nm f=0.0020 <S**2>=0.000
270 ->276 0.41376
271 ->276 0.57019

Excited State 27: Singlet-E 1.5171 eV 817.25 nm f=0.0020 <S**2>=0.000
270 ->276 0.57019
271 ->276 -0.41376

Excited State 28: Singlet-A 1.5172 eV 817.21 nm f=0.0000 <S**2>=0.000
269 ->276 0.70417

Excited State 29: Singlet-B 1.5859 eV 781.78 nm f=0.0318 <S**2>=0.000
272 ->276 -0.10783
273 ->276 0.67221

Excited State 30: Singlet-A 1.6353 eV 758.18 nm f=0.0000 <S**2>=0.000
268 ->276 0.67757

Excited State 31: Singlet-E 1.6466 eV 752.97 nm f=0.0361 <S**2>=0.000
261 ->275 0.14051
266 ->276 0.66988

Excited State 32: Singlet-E 1.6466 eV 752.97 nm f=0.0361 <S**2>=0.000
261 ->274 -0.14051
267 ->276 0.66988

Excited State 33: Singlet-E 1.7917 eV 691.98 nm f=0.1938 <S**2>=0.000

256 ->275 0.16129
260 ->275 -0.15733
261 ->274 -0.35812
261 ->275 0.52200
266 ->276 -0.13515

Excited State 34: Singlet-E 1.7917 eV 691.98 nm f=0.1938 <S**2>=0.000
256 ->274 0.16129
260 ->274 0.15733
261 ->274 0.52200
261 ->275 0.35812
267 ->276 0.13515

Excited State 35: Singlet-B 1.8998 eV 652.60 nm f=0.0004 <S**2>=0.000
258 ->274 0.14453
258 ->275 -0.11385
259 ->274 0.11386
259 ->275 0.14450
265 ->276 0.65562

Excited State 36: Singlet-E 1.9039 eV 651.21 nm f=0.0753 <S**2>=0.000
260 ->274 -0.37683
260 ->275 0.46488
261 ->275 0.15922
263 ->276 -0.32643

Excited State 37: Singlet-E 1.9039 eV 651.21 nm f=0.0752 <S**2>=0.000
260 ->274 0.46488
260 ->275 0.37683
261 ->274 -0.15922
262 ->276 0.32643

Excited State 38: Singlet-A 1.9148 eV 647.49 nm f=0.0000 <S**2>=0.000
258 ->275 0.16918
259 ->274 0.16915
264 ->276 0.65290

Excited state symmetry could not be determined.
Excited State 39: Singlet-?Sym 1.9286 eV 642.87 nm f=0.0048 <S**2>=0.000
258 ->274 0.47080
258 ->275 0.11191
259 ->274 -0.11196
259 ->275 0.47079
265 ->276 -0.16643

Excited State 40: Singlet-E 1.9366 eV 640.22 nm f=0.0346 <S**2>=0.000
260 ->275 0.31127
262 ->276 -0.23527
263 ->276 0.57234

Excited State 41: Singlet-E 1.9366 eV 640.22 nm f=0.0346 <S**2>=0.000
260 ->274 -0.31127
262 ->276 0.57234
263 ->276 0.23527

Excited state symmetry could not be determined.
Excited State 42: Singlet-?Sym 1.9386 eV 639.57 nm f=0.0000 <S**2>=0.000
258 ->274 -0.48790
259 ->275 0.48793
264 ->276 0.13806

Excited state symmetry could not be determined.
Excited State 43: Singlet-?Sym 1.9987 eV 620.32 nm f=0.0292 <S**2>=0.000
258 ->275 0.46280
259 ->274 -0.46271
265 ->276 0.18673

Excited State 44: Singlet-E 2.0097 eV 616.93 nm f=0.0002 <S**2>=0.000
257 ->274 -0.62474
257 ->275 0.32825

Excited State 45: Singlet-E 2.0097 eV 616.93 nm f=0.0002 <S**2>=0.000
257 ->274 0.32825
257 ->275 0.62474

Excited state symmetry could not be determined.
Excited State 46: Singlet-?Sym 2.0127 eV 616.01 nm f=0.0000 <S**2>=0.000
258 ->275 0.45428
259 ->274 0.45437
260 ->276 -0.10185
264 ->276 -0.21927
268 ->276 0.10047

Excited State 47: Singlet-E 2.2843 eV 542.78 nm f=0.0309 <S**2>=0.000
249 ->275 -0.11800
252 ->275 0.14220
253 ->274 -0.10905
253 ->275 0.50429
256 ->274 -0.11069
256 ->275 -0.41418

Excited State 48: Singlet-E 2.2843 eV 542.78 nm f=0.0309 <S**2>=0.000
249 ->274 -0.11801
252 ->274 -0.14220
253 ->274 0.50429
253 ->275 0.10905
256 ->274 -0.41418
256 ->275 0.11069

Excited state symmetry could not be determined.
Excited State 49: Singlet-?Sym 2.2929 eV 540.73 nm f=0.0000 <S**2>=0.000
254 ->275 -0.49546
255 ->274 0.49581

Excited state symmetry could not be determined.
Excited State 50: Singlet-?Sym 2.2930 eV 540.70 nm f=0.0008 <S**2>=0.000
254 ->274 -0.32429
254 ->275 0.37934
255 ->274 0.37886
255 ->275 0.32428

Excited State 51: Singlet-E 2.3014 eV 538.74 nm f=0.0011 <S**2>=0.000
252 ->274 0.58596
252 ->275 -0.35958
253 ->275 0.11113

Excited State 52: Singlet-E 2.3014 eV 538.74 nm f=0.0011 <S**2>=0.000
252 ->274 0.35958
252 ->275 0.58596
253 ->274 0.11113

Excited state symmetry could not be determined.
Excited State 53: Singlet-?Sym 2.3029 eV 538.39 nm f=0.0000 <S**2>=0.000
254 ->274 -0.37745
254 ->275 -0.32225
255 ->274 -0.32283
255 ->275 0.38229

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 2.3031 eV 538.33 nm f=0.0000 <S**2>=0.000
254 ->274 0.49658
255 ->275 0.49283

Excited State 55: Singlet-E 2.3810 eV 520.72 nm f=0.0681 <S**2>=0.000
249 ->274 0.26566

253 ->275 0.42719
256 ->274 0.12946
256 ->275 0.43977
261 ->275 -0.10023

Excited State 56: Singlet-E 2.3810 eV 520.72 nm f=0.0681 <S**2>=0.000
249 ->275 -0.26566
253 ->274 0.42719
256 ->274 0.43977
256 ->275 -0.12947
261 ->274 -0.10023

Excited state symmetry could not be determined.
Excited State 57: Singlet-?Sym 2.4227 eV 511.77 nm f=0.0000 <S**2>=0.000
250 ->274 -0.11510
250 ->275 -0.48648
251 ->274 0.48649
251 ->275 -0.11512

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 2.4297 eV 510.28 nm f=0.0000 <S**2>=0.000
250 ->274 0.45347
250 ->275 0.21027
251 ->274 0.21025
251 ->275 -0.45346

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 2.5082 eV 494.31 nm f=0.0004 <S**2>=0.000
250 ->274 -0.20611
250 ->275 0.44355
251 ->274 0.44353
251 ->275 0.20603
257 ->276 -0.12102

Excited state symmetry could not be determined.
Excited State 60: Singlet-?Sym 2.5111 eV 493.75 nm f=0.0000 <S**2>=0.000
250 ->274 0.48213
250 ->275 -0.11402
251 ->274 0.11408
251 ->275 0.48217

Excited State 61: Singlet-A 2.5217 eV 491.67 nm f=0.0000 <S**2>=0.000
269 ->280 -0.10689
272 ->281 -0.11026
273 ->277 0.65997

Excited State 62: Singlet-A 2.5381 eV 488.49 nm f=0.0000 <S**2>=0.000
272 ->277 0.67663
273 ->281 0.12572

Excited State 63: Singlet-E 2.5390 eV 488.32 nm f=0.0000 <S**2>=0.000
270 ->277 -0.14889
271 ->277 0.66091

Excited State 64: Singlet-E 2.5390 eV 488.32 nm f=0.0000 <S**2>=0.000
270 ->277 0.66091
271 ->277 0.14889

Excited State 65: Singlet-B 2.5396 eV 488.20 nm f=0.0000 <S**2>=0.000
269 ->277 0.67860
273 ->280 0.12583

Excited State 66: Singlet-E 2.5684 eV 482.73 nm f=0.0033 <S**2>=0.000
269 ->283 -0.12222
271 ->280 -0.12000
271 ->281 -0.12853
272 ->278 -0.13177
273 ->278 0.27573
273 ->279 0.55887

Excited State 67: Singlet-E 2.5684 eV 482.73 nm f=0.0033 <S**2>=0.000
269 ->282 -0.12222
270 ->280 -0.12000
270 ->281 0.12852
272 ->279 0.13177
273 ->278 0.55887
273 ->279 -0.27573

Excited State 68: Singlet-B 2.5763 eV 481.25 nm f=0.0035 <S**2>=0.000
261 ->276 0.12207
268 ->277 0.61401
269 ->281 -0.13423
270 ->279 0.11870
270 ->282 0.12156
271 ->278 -0.11869
271 ->283 -0.12156
272 ->280 -0.13382

Excited State 69: Singlet-B 2.5892 eV 478.84 nm f=0.0512 <S**2>=0.000
261 ->276 0.63975

268 ->277 -0.18112

Excited state symmetry could not be determined.
Excited State 70: Singlet-?Sym 2.5913 eV 478.47 nm f=0.0002 <S**2>=0.000
268 ->281 0.13319
270 ->278 0.44722
271 ->279 0.44736
273 ->280 0.21096

Excited State 71: Singlet-E 2.5915 eV 478.42 nm f=0.0002 <S**2>=0.000
268 ->282 -0.12654
269 ->278 0.38416
269 ->279 0.23429
272 ->278 -0.16266
272 ->279 0.39634
273 ->283 0.21205

Excited State 72: Singlet-E 2.5915 eV 478.42 nm f=0.0002 <S**2>=0.000
268 ->283 0.12654
269 ->278 -0.23429
269 ->279 0.38415
272 ->278 0.39634
272 ->279 0.16266
273 ->282 -0.21205

Excited state symmetry could not be determined.
Excited State 73: Singlet-?Sym 2.5931 eV 478.13 nm f=0.0000 <S**2>=0.000
268 ->280 -0.13900
270 ->278 0.41702
270 ->279 -0.16049
271 ->278 -0.16046
271 ->279 -0.41688
273 ->281 -0.21837

Excited State 74: Singlet-E 2.5981 eV 477.22 nm f=0.0038 <S**2>=0.000
267 ->277 -0.10388
269 ->278 0.46757
272 ->278 0.41032
272 ->279 -0.26136
273 ->278 0.10464
273 ->279 0.10323

Excited State 75: Singlet-E 2.5981 eV 477.22 nm f=0.0038 <S**2>=0.000
266 ->277 0.10388
269 ->279 0.46757

272 ->278 -0.26136
272 ->279 -0.41032
273 ->278 0.10323
273 ->279 -0.10464

Excited state symmetry could not be determined.
Excited State 76: Singlet-?Sym 2.5987 eV 477.10 nm f=0.0060 <S**2>=0.000
261 ->276 0.17241
268 ->277 0.13786
270 ->279 -0.47139
271 ->278 0.47142

Excited state symmetry could not be determined.
Excited State 77: Singlet-?Sym 2.6003 eV 476.81 nm f=0.0000 <S**2>=0.000
270 ->278 0.17912
270 ->279 0.46259
271 ->278 0.46256
271 ->279 -0.17910

Excited State 78: Singlet-E 2.6094 eV 475.15 nm f=0.0119 <S**2>=0.000
267 ->277 0.61298
269 ->278 0.14982
271 ->280 -0.10795
271 ->281 -0.11053
273 ->279 -0.14909

Excited State 79: Singlet-E 2.6094 eV 475.15 nm f=0.0119 <S**2>=0.000
266 ->277 0.61298
269 ->279 -0.14982
270 ->280 0.10795
270 ->281 -0.11053
273 ->278 0.14909

Excited State 80: Singlet-E 2.6329 eV 470.90 nm f=0.0018 <S**2>=0.000
267 ->277 -0.18967
268 ->278 0.29285
268 ->279 0.57439
273 ->279 -0.10117

Excited State 81: Singlet-E 2.6329 eV 470.90 nm f=0.0018 <S**2>=0.000
266 ->277 -0.18967
268 ->278 0.57439
268 ->279 -0.29285
273 ->278 0.10117

Excited state symmetry could not be determined.
Excited State 82: Singlet-?Sym 2.6484 eV 468.15 nm f=0.0000 <S**2>=0.000
266 ->278 -0.37149
266 ->279 0.20734
267 ->278 0.20752
267 ->279 0.37200
269 ->280 -0.16562
270 ->282 -0.12713
270 ->283 -0.10404
271 ->282 0.10412
271 ->283 -0.12731
272 ->281 -0.16542
273 ->277 -0.12855

Excited state symmetry could not be determined.
Excited State 83: Singlet-?Sym 2.6503 eV 467.80 nm f=0.0094 <S**2>=0.000
261 ->276 -0.12204
266 ->278 0.38987
266 ->279 -0.12076
267 ->278 0.12047
267 ->279 0.38939
268 ->277 -0.15266
269 ->281 -0.16478
270 ->282 0.14901
271 ->283 -0.14885
272 ->280 -0.16700

Excited state symmetry could not be determined.
Excited State 84: Singlet-?Sym 2.6734 eV 463.77 nm f=0.0005 <S**2>=0.000
266 ->278 0.12549
266 ->279 0.47947
267 ->278 -0.47947
267 ->279 0.12552

Excited state symmetry could not be determined.
Excited State 85: Singlet-?Sym 2.6743 eV 463.61 nm f=0.0000 <S**2>=0.000
266 ->278 0.21002
266 ->279 0.44589
267 ->278 0.44588
267 ->279 -0.20999

Excited State 86: Singlet-E 2.7395 eV 452.58 nm f=0.0441 <S**2>=0.000
245 ->274 -0.14942
248 ->274 0.56464
248 ->275 0.35609

258 ->276 -0.12841

Excited State 87: Singlet-E 2.7395 eV 452.58 nm f=0.0441 <S**2>=0.000
245 ->275 0.14942
248 ->274 -0.35609
248 ->275 0.56464
259 ->276 0.12842

Excited state symmetry could not be determined.
Excited State 88: Singlet-?Sym 2.7468 eV 451.38 nm f=0.0000 <S**2>=0.000
246 ->274 0.22983
246 ->275 0.43899
247 ->274 0.43891
247 ->275 -0.23002

Excited state symmetry could not be determined.
Excited State 89: Singlet-?Sym 2.7500 eV 450.85 nm f=0.0000 <S**2>=0.000
246 ->274 0.41835
246 ->275 -0.23393
247 ->274 0.23411
247 ->275 0.41825
260 ->276 -0.11644
273 ->281 0.11492

Excited State 90: Singlet-B 2.7524 eV 450.46 nm f=0.0000 <S**2>=0.000
268 ->281 -0.13155
270 ->282 0.11668
270 ->283 -0.10319
271 ->282 -0.10319
271 ->283 -0.11667
272 ->284 0.20137
273 ->280 0.56672

Excited State 91: Singlet-E 2.7548 eV 450.07 nm f=0.0005 <S**2>=0.000
268 ->283 -0.14398
269 ->283 -0.11146
271 ->284 0.19366
272 ->282 -0.12648
273 ->282 -0.47209
273 ->283 0.33300

Excited State 92: Singlet-E 2.7548 eV 450.07 nm f=0.0005 <S**2>=0.000
268 ->282 0.14398
269 ->282 0.11146
270 ->284 -0.19365

272 ->283 0.12648
273 ->282 0.33300
273 ->283 0.47209

Excited State 93: Singlet-A 2.7560 eV 449.87 nm f=0.0000 <S**2>=0.000
268 ->280 -0.16745
269 ->284 0.21941
273 ->281 0.58432

Excited State 94: Singlet-B 2.7643 eV 448.53 nm f=0.0029 <S**2>=0.000
246 ->274 0.27076
246 ->275 -0.12575
247 ->274 -0.12596
247 ->275 -0.27065
266 ->278 0.11868
267 ->279 0.11867
272 ->280 0.40167
273 ->284 -0.32712

Excited State 95: Singlet-A 2.7655 eV 448.32 nm f=0.0000 <S**2>=0.000
269 ->280 0.51497
270 ->282 -0.17475
271 ->283 -0.17477
272 ->281 -0.37439

Excited State 96: Singlet-B 2.7657 eV 448.28 nm f=0.0013 <S**2>=0.000
246 ->274 -0.19010
247 ->275 0.18989
269 ->281 -0.18866
270 ->283 0.25429
271 ->282 0.25434
272 ->280 0.41630
273 ->284 0.20141

Excited State 97: Singlet-E 2.7660 eV 448.25 nm f=0.0000 <S**2>=0.000
269 ->282 -0.22432
270 ->280 0.18865
270 ->281 0.13449
271 ->280 -0.54247
272 ->282 -0.17564
272 ->283 0.24692

Excited State 98: Singlet-E 2.7660 eV 448.25 nm f=0.0000 <S**2>=0.000
269 ->283 -0.22432
270 ->280 0.54247

271 ->280 0.18865
271 ->281 -0.13448
272 ->282 0.24692
272 ->283 0.17564

Excited State 99: Singlet-E 2.7664 eV 448.17 nm f=0.0003 <S**2>=0.000
269 ->282 0.18842
269 ->283 -0.12477
270 ->281 0.32860
271 ->280 0.16811
271 ->281 -0.31525
272 ->282 -0.42667
272 ->283 0.13064

Excited State 100: Singlet-E 2.7664 eV 448.17 nm f=0.0003 <S**2>=0.000
269 ->282 -0.12477
269 ->283 -0.18841
270 ->280 0.16810
270 ->281 0.31526
271 ->281 0.32859
272 ->282 -0.13064
272 ->283 -0.42668

Excited state symmetry could not be determined.
Excited State 101: Singlet-?Sym 2.7668 eV 448.11 nm f=0.0000 <S**2>=0.000
269 ->280 -0.29010
270 ->282 -0.13436
270 ->283 0.43183
271 ->282 -0.43181
271 ->283 -0.13437

Excited State 102: Singlet-A 2.7669 eV 448.10 nm f=0.0000 <S**2>=0.000
269 ->280 0.13378
270 ->282 -0.34724
271 ->283 -0.34722
272 ->281 0.47044

Excited State 103: Singlet-B 2.7674 eV 448.02 nm f=0.0000 <S**2>=0.000
269 ->281 0.56211
270 ->282 0.29114
271 ->283 -0.29119

Excited state symmetry could not be determined.
Excited State 104: Singlet-?Sym 2.7682 eV 447.88 nm f=0.0000 <S**2>=0.000
246 ->274 0.20688

246 ->275 0.42408
247 ->274 -0.42400
247 ->275 0.20703
260 ->276 -0.18967

Excited State 105: Singlet-E 2.7685 eV 447.84 nm f=0.0016 <S**2>=0.000
269 ->282 0.49048
270 ->281 0.29933
271 ->281 0.20203
272 ->282 0.21582
272 ->283 0.10955
273 ->282 -0.12811

Excited State 106: Singlet-E 2.7685 eV 447.84 nm f=0.0016 <S**2>=0.000
269 ->283 0.49048
270 ->281 0.20202
271 ->281 -0.29934
272 ->282 0.10955
272 ->283 -0.21581
273 ->283 0.12810

Excited state symmetry could not be determined.
Excited State 107: Singlet-?Sym 2.7702 eV 447.57 nm f=0.0002 <S**2>=0.000
268 ->281 -0.13357
269 ->281 0.11676
270 ->282 -0.19683
270 ->283 0.37932
271 ->282 0.37932
271 ->283 0.19684
272 ->280 -0.18470
272 ->284 0.11497
273 ->280 0.17683

Excited State 108: Singlet-E 2.7704 eV 447.53 nm f=0.0710 <S**2>=0.000
245 ->274 -0.37535
245 ->275 0.46443
249 ->274 0.24111
258 ->276 0.17010

Excited State 109: Singlet-E 2.7704 eV 447.53 nm f=0.0709 <S**2>=0.000
245 ->274 0.46443
245 ->275 0.37535
249 ->275 -0.24110
259 ->276 -0.17011

Excited State 110: Singlet-B 2.7884 eV 444.64 nm f=0.0010 <S**2>=0.000
246 ->274 0.27256
246 ->275 -0.15878
247 ->274 -0.15866
247 ->275 -0.27263
273 ->284 0.49732

Excited State 111: Singlet-B 2.7944 eV 443.69 nm f=0.0000 <S**2>=0.000
266 ->282 -0.10341
267 ->283 0.10343
268 ->281 0.38056
272 ->284 0.53724

Excited State 112: Singlet-A 2.7954 eV 443.54 nm f=0.0000 <S**2>=0.000
260 ->276 -0.15777
268 ->280 0.40361
269 ->284 0.49623

Excited State 113: Singlet-E 2.7957 eV 443.47 nm f=0.0003 <S**2>=0.000
268 ->283 0.39148
270 ->284 0.40242
271 ->284 0.34175

Excited State 114: Singlet-E 2.7957 eV 443.47 nm f=0.0003 <S**2>=0.000
268 ->282 -0.39148
270 ->284 -0.34175
271 ->284 0.40242

Excited State 115: Singlet-A 2.7994 eV 442.90 nm f=0.0000 <S**2>=0.000
260 ->276 0.44924
265 ->277 -0.16290
266 ->278 -0.11428
267 ->279 0.11428
268 ->280 0.11081
268 ->284 -0.31291
269 ->280 0.10886
269 ->284 0.15503
270 ->282 0.10315
271 ->283 0.10319
272 ->281 0.12258

Excited State 116: Singlet-E 2.8157 eV 440.33 nm f=0.0393 <S**2>=0.000
245 ->274 -0.14568
248 ->274 -0.10792
249 ->275 -0.14548

258 ->276 -0.42203
259 ->276 0.15338
262 ->277 -0.12226
266 ->284 0.22079
267 ->280 -0.14592
267 ->284 -0.14399
268 ->282 -0.10308
269 ->282 -0.11440
270 ->281 0.11426

Excited State 117: Singlet-E 2.8157 eV 440.33 nm f=0.0393 <S**2>=0.000
245 ->275 0.14568
248 ->275 -0.10792
249 ->274 -0.14548
258 ->276 0.15338
259 ->276 0.42202
263 ->277 -0.12226
266 ->280 -0.14592
266 ->284 -0.14399
267 ->284 -0.22079
268 ->283 0.10308
269 ->283 0.11440
271 ->281 0.11426

Excited State 118: Singlet-A 2.8227 eV 439.24 nm f=0.0000 <S**2>=0.000
266 ->282 -0.29429
266 ->283 -0.20712
267 ->282 0.20713
267 ->283 -0.29432
268 ->280 0.43949
269 ->284 -0.19389

Excited State 119: Singlet-B 2.8232 eV 439.16 nm f=0.0000 <S**2>=0.000
266 ->282 0.31496
266 ->283 0.16881
267 ->282 0.16879
267 ->283 -0.31493
268 ->281 0.45859
272 ->284 -0.15799

Excited State 120: Singlet-E 2.8232 eV 439.16 nm f=0.0068 <S**2>=0.000
259 ->276 0.12304
266 ->280 0.19142
266 ->281 -0.15371
267 ->280 0.27813

267 ->281 0.29690
268 ->283 -0.43747
271 ->284 0.13297

Excited State 121: Singlet-E 2.8232 eV 439.16 nm f=0.0068 <S**2>=0.000
258 ->276 0.12304
266 ->280 0.27813
266 ->281 -0.29690
267 ->280 -0.19142
267 ->281 -0.15371
268 ->282 -0.43746
270 ->284 0.13297

Excited State 122: Singlet-E 2.8383 eV 436.83 nm f=0.0055 <S**2>=0.000
266 ->280 0.26104
266 ->281 0.22697
267 ->280 0.39312
267 ->281 -0.45235

Excited State 123: Singlet-E 2.8383 eV 436.83 nm f=0.0055 <S**2>=0.000
266 ->280 -0.39312
266 ->281 -0.45235
267 ->280 0.26105
267 ->281 -0.22697

Excited state symmetry could not be determined.
Excited State 124: Singlet-?Sym 2.8395 eV 436.64 nm f=0.0000 <S**2>=0.000
260 ->276 0.15983
266 ->282 -0.27351
266 ->283 0.39336
267 ->282 -0.39352
267 ->283 -0.27360

Excited state symmetry could not be determined.
Excited State 125: Singlet-?Sym 2.8396 eV 436.62 nm f=0.0000 <S**2>=0.000
266 ->282 -0.23544
266 ->283 0.44031
267 ->282 0.44016
267 ->283 0.23533

Excited State 126: Singlet-E 2.8473 eV 435.45 nm f=0.1357 <S**2>=0.000
245 ->274 0.21457
248 ->274 0.13103
249 ->275 0.22702
259 ->276 0.28882

263 ->277 0.18063
265 ->278 0.16130
266 ->284 0.23363
267 ->280 0.12331
267 ->284 0.17032
270 ->280 -0.10389
272 ->282 0.11316

Excited State 127: Singlet-E 2.8473 eV 435.45 nm f=0.1357 <S**2>=0.000
245 ->275 -0.21457
248 ->275 0.13103
249 ->274 0.22702
258 ->276 0.28881
262 ->277 -0.18062
265 ->279 -0.16128
266 ->280 0.12332
266 ->284 0.17032
267 ->284 -0.23363
271 ->280 0.10389
272 ->283 0.11316

Excited State 128: Singlet-A 2.8494 eV 435.12 nm f=0.0000 <S**2>=0.000
260 ->276 0.39429
266 ->278 0.10466
267 ->279 -0.10469
268 ->284 0.44916

Excited State 129: Singlet-B 2.8757 eV 431.15 nm f=0.0007 <S**2>=0.000
241 ->275 0.12060
242 ->274 0.12061
257 ->276 0.66672

Excited State 130: Singlet-A 2.8762 eV 431.07 nm f=0.0000 <S**2>=0.000
260 ->276 0.10049
262 ->279 0.16228
263 ->278 0.16224
265 ->277 0.54691
268 ->284 -0.32162

Excited State 131: Singlet-E 2.8780 eV 430.79 nm f=0.0027 <S**2>=0.000
244 ->274 0.65023
244 ->275 0.20682

Excited State 132: Singlet-E 2.8780 eV 430.79 nm f=0.0027 <S**2>=0.000
244 ->274 0.20682

244 ->275 -0.65023

Excited State 133: Singlet-B 2.8792 eV 430.62 nm f=0.0002 <S**2>=0.000
262 ->278 0.17823
262 ->279 0.14575
263 ->278 -0.14573
263 ->279 0.17823
264 ->277 0.53553
269 ->281 -0.10651
272 ->280 -0.10225
273 ->284 -0.14413

Excited State 134: Singlet-E 2.8961 eV 428.11 nm f=0.0059 <S**2>=0.000
262 ->277 -0.14851
263 ->277 -0.40419
264 ->279 -0.17499
265 ->278 -0.16438
265 ->279 -0.14456
266 ->284 0.19929
267 ->284 0.39559

Excited State 135: Singlet-E 2.8961 eV 428.11 nm f=0.0059 <S**2>=0.000
262 ->277 0.40419
263 ->277 -0.14851
264 ->278 0.17498
265 ->278 -0.14458
265 ->279 0.16435
266 ->284 0.39560
267 ->284 -0.19929

Excited State 136: Singlet-E 2.9059 eV 426.67 nm f=0.0046 <S**2>=0.000
243 ->274 0.62002
243 ->275 -0.10090
266 ->284 0.11858
271 ->284 0.10023

Excited State 137: Singlet-E 2.9059 eV 426.67 nm f=0.0046 <S**2>=0.000
243 ->274 0.10090
243 ->275 0.62002
267 ->284 0.11858
270 ->284 -0.10023

Excited state symmetry could not be determined.
Excited State 138: Singlet-?Sym 2.9146 eV 425.40 nm f=0.0002 <S**2>=0.000
241 ->274 0.36773

241 ->275 0.12057
242 ->274 0.12032
242 ->275 -0.36895
262 ->282 0.10995
263 ->283 -0.10992
264 ->281 -0.12162
265 ->280 -0.12402
266 ->282 0.14514
267 ->283 -0.14470
268 ->281 -0.13655
272 ->284 0.19585

Excited state symmetry could not be determined.
Excited State 139: Singlet-?Sym 2.9148 eV 425.36 nm f=0.0000 <S**2>=0.000
241 ->274 0.37002
241 ->275 -0.11150
242 ->274 0.11190
242 ->275 0.36882
262 ->283 -0.12146
263 ->282 0.12132
264 ->280 -0.12447
265 ->281 -0.12603
266 ->282 -0.13728
266 ->283 -0.10025
267 ->282 0.10049
267 ->283 -0.13776
268 ->280 -0.13723
269 ->284 0.20370

Excited state symmetry could not be determined.
Excited State 140: Singlet-?Sym 2.9206 eV 424.51 nm f=0.0000 <S**2>=0.000
241 ->275 -0.48643
242 ->274 0.48648

Excited state symmetry could not be determined.
Excited State 141: Singlet-?Sym 2.9241 eV 424.00 nm f=0.0001 <S**2>=0.000
241 ->274 -0.24240
241 ->275 0.40880
242 ->274 0.40870
242 ->275 0.24241
257 ->276 -0.14790

Excited State 142: Singlet-E 2.9467 eV 420.75 nm f=0.0043 <S**2>=0.000
243 ->275 -0.22780
244 ->274 -0.12057

262 ->281 -0.21530
263 ->280 -0.22283
264 ->282 0.22185
265 ->283 -0.21832
266 ->280 0.12679
266 ->281 -0.14437
267 ->280 -0.12340
267 ->281 -0.10309
268 ->282 0.15870
270 ->284 -0.16620
271 ->284 0.18410
273 ->283 -0.11850

Excited State 143: Singlet-E 2.9467 eV 420.75 nm f=0.0043 <S**2>=0.000
243 ->274 -0.22780
244 ->275 -0.12058
262 ->280 -0.22283
263 ->281 -0.21530
264 ->283 -0.22185
265 ->282 0.21832
266 ->280 -0.12341
266 ->281 0.10309
267 ->280 -0.12679
267 ->281 -0.14437
268 ->283 -0.15870
270 ->284 0.18411
271 ->284 0.16620
273 ->282 0.11849

Excited State 144: Singlet-E 2.9542 eV 419.69 nm f=0.0084 <S**2>=0.000
262 ->277 0.45080
263 ->277 -0.13005
264 ->278 -0.19801
264 ->279 -0.10318
265 ->278 0.30249
265 ->279 -0.33381
266 ->284 -0.10484

Excited State 145: Singlet-E 2.9542 eV 419.69 nm f=0.0084 <S**2>=0.000
262 ->277 0.13004
263 ->277 0.45079
264 ->278 0.10318
264 ->279 -0.19793
265 ->278 -0.33382
265 ->279 -0.30255

267 ->284 0.10484

Excited state symmetry could not be determined.
Excited State 146: Singlet-?Sym 2.9553 eV 419.54 nm f=0.0002 <S**2>=0.000
241 ->274 0.22820
241 ->275 0.22394
242 ->274 0.22401
242 ->275 -0.22743
262 ->282 -0.18042
263 ->283 0.18046
264 ->281 0.20027
265 ->280 0.20763
266 ->282 -0.11983
267 ->283 0.12012
268 ->281 0.12524
272 ->284 -0.19755

Excited state symmetry could not be determined.
Excited State 147: Singlet-?Sym 2.9555 eV 419.50 nm f=0.0000 <S**2>=0.000
241 ->274 0.31085
242 ->275 0.31142
262 ->283 0.19848
263 ->282 -0.19869
264 ->280 0.20522
265 ->281 0.20957
266 ->282 0.11416
267 ->283 0.11387
268 ->280 0.12637
269 ->284 -0.20408
273 ->281 0.10020

Excited state symmetry could not be determined.
Excited State 148: Singlet-?Sym 2.9622 eV 418.56 nm f=0.0000 <S**2>=0.000
262 ->278 -0.15031
262 ->279 0.38542
263 ->278 0.38541
263 ->279 0.15029
265 ->277 -0.35506

Excited State 149: Singlet-B 2.9633 eV 418.40 nm f=0.0001 <S**2>=0.000
262 ->278 -0.29821
262 ->279 -0.24838
263 ->278 0.24839
263 ->279 -0.29821
264 ->277 0.41964

Excited State 150: Singlet-E 2.9849 eV 415.37 nm f=0.0326 <S**2>=0.000
264 ->278 0.10171
264 ->279 0.56451
265 ->279 -0.35105

Table S3: Vertical Excitation Energies of TAP^{Fc}Mg using BP86 PCM-TDDFT
Excited State 1: Singlet-E 0.8626 eV 1437.29 nm f=0.0071 <S**2>=0.000
245 ->250 0.19295
245 ->251 -0.13653
248 ->250 0.38487
248 ->251 -0.18985
249 ->250 0.48107
249 ->251 0.12163
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3090.88940867
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-E 0.8626 eV 1437.29 nm f=0.0071 <S**2>=0.000
245 ->250 0.13654
245 ->251 0.19296
248 ->250 -0.18984
248 ->251 -0.38487
249 ->250 -0.12163
249 ->251 0.48106

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 0.8774 eV 1413.07 nm f=0.0000 <S**2>=0.000
246 ->250 -0.12082
246 ->251 -0.48368
247 ->250 0.48370
247 ->251 -0.12083

Excited state symmetry could not be determined.
Excited State 4: Singlet-?Sym 0.8812 eV 1407.07 nm f=0.0000 <S**2>=0.000
246 ->250 -0.16173
246 ->251 0.46305
247 ->250 0.46305
247 ->251 0.16185

Excited State 5: Singlet-E 0.8815 eV 1406.58 nm f=0.0009 <S**2>=0.000
244 ->250 -0.27192
245 ->250 0.48230
245 ->251 0.25419
248 ->250 0.13884
248 ->251 0.31285

Excited State 6: Singlet-E 0.8815 eV 1406.58 nm f=0.0009 <S**2>=0.000
244 ->251 0.27192
245 ->250 -0.25420
245 ->251 0.48232
248 ->250 0.31283
248 ->251 -0.13881

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 0.8836 eV 1403.22 nm f=0.0000 <S**2>=0.000
242 ->250 -0.13249
243 ->251 -0.13253
246 ->250 0.46419
246 ->251 -0.10720
247 ->250 0.10708
247 ->251 0.46419

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 0.8858 eV 1399.76 nm f=0.0002 <S**2>=0.000
242 ->250 -0.20514
243 ->251 0.20513
246 ->250 0.43781
246 ->251 0.12568
247 ->250 0.12568
247 ->251 -0.43777

Excited State 9: Singlet-E 0.8860 eV 1399.32 nm f=0.0019 <S**2>=0.000
244 ->250 -0.33832
244 ->251 0.42084
245 ->251 -0.35671
248 ->250 0.11922
248 ->251 -0.16734
249 ->250 -0.16971

Excited State 10: Singlet-E 0.8860 eV 1399.32 nm f=0.0019 <S**2>=0.000
244 ->250 0.42083
244 ->251 0.33833
245 ->250 0.35673
248 ->250 -0.16733

248 ->251 -0.11918
249 ->251 -0.16971

Excited state symmetry could not be determined.
Excited State 11: Singlet-?Sym 0.9091 eV 1363.87 nm f=0.0000 <S**2>=0.000
242 ->250 0.16954
242 ->251 0.46872
243 ->250 -0.46871
243 ->251 0.16954

Excited state symmetry could not be determined.
Excited State 12: Singlet-?Sym 0.9184 eV 1350.05 nm f=0.0000 <S**2>=0.000
242 ->251 0.48817
243 ->250 0.48818

Excited State 13: Singlet-E 1.0319 eV 1201.47 nm f=0.1828 <S**2>=0.000
244 ->250 -0.31525
244 ->251 0.13566
248 ->250 -0.39097
249 ->250 0.44551

Excited State 14: Singlet-E 1.0320 eV 1201.45 nm f=0.1828 <S**2>=0.000
244 ->250 0.13565
244 ->251 0.31523
248 ->251 0.39096
249 ->251 0.44552

Excited state symmetry could not be determined.
Excited State 15: Singlet-?Sym 1.0417 eV 1190.20 nm f=0.0229 <S**2>=0.000
242 ->250 0.44188
243 ->251 -0.44175
246 ->250 0.17684
246 ->251 0.11487
247 ->250 0.11488
247 ->251 -0.17680

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 1.1019 eV 1125.17 nm f=0.0000 <S**2>=0.000
242 ->250 0.44133
242 ->251 -0.15024
243 ->250 0.15026
243 ->251 0.44146
246 ->250 0.13610
247 ->251 0.13615

Excited State 17: Singlet-E 1.2977 eV 955.43 nm f=0.0020 <S**2>=0.000
240 ->250 0.46786
240 ->251 -0.10618
241 ->250 0.50081
241 ->251 -0.12790

Excited State 18: Singlet-E 1.2977 eV 955.43 nm f=0.0020 <S**2>=0.000
240 ->250 -0.10619
240 ->251 -0.46788
241 ->250 0.12789
241 ->251 0.50079

Excited state symmetry could not be determined.
Excited State 19: Singlet-?Sym 1.3025 eV 951.93 nm f=0.0000 <S**2>=0.000
238 ->250 0.11100
238 ->251 0.48740
239 ->250 0.48749
239 ->251 -0.11102

Excited state symmetry could not be determined.
Excited State 20: Singlet-?Sym 1.3036 eV 951.08 nm f=0.0000 <S**2>=0.000
238 ->250 0.11750
238 ->251 0.48588
239 ->250 -0.48579
239 ->251 0.11747

Excited State 21: Singlet-E 1.3328 eV 930.22 nm f=0.0297 <S**2>=0.000
240 ->250 0.50416
240 ->251 -0.11094
241 ->250 -0.45701
241 ->251 0.11860

Excited State 22: Singlet-E 1.3328 eV 930.22 nm f=0.0297 <S**2>=0.000
240 ->250 0.11093
240 ->251 0.50415
241 ->250 0.11861
241 ->251 0.45703

Excited state symmetry could not be determined.
Excited State 23: Singlet-?Sym 1.3373 eV 927.15 nm f=0.0031 <S**2>=0.000
238 ->250 0.48361
238 ->251 -0.11655
239 ->250 0.11650
239 ->251 0.48338

Excited state symmetry could not be determined.
Excited State 24: Singlet-?Sym 1.3458 eV 921.28 nm f=0.0000 <S**2>=0.000
238 ->250 -0.47908
238 ->251 0.10862
239 ->250 0.10868
239 ->251 0.47931

Excited State 25: Singlet-E 1.9552 eV 634.11 nm f=0.1941 <S**2>=0.000
229 ->250 -0.10508
232 ->250 0.10628
232 ->251 0.12337
236 ->251 -0.19378
237 ->250 0.22332
237 ->251 0.56421
243 ->252 0.17730

Excited State 26: Singlet-E 1.9552 eV 634.11 nm f=0.1942 <S**2>=0.000
229 ->251 0.10508
232 ->250 0.12338
232 ->251 -0.10629
236 ->250 0.19377
237 ->250 0.56421
237 ->251 -0.22332
242 ->252 -0.17729

Excited State 27: Singlet-B 1.9799 eV 626.22 nm f=0.0124 <S**2>=0.000
234 ->250 -0.11518
235 ->251 0.11518
245 ->252 0.25778
249 ->252 0.62982

Excited State 28: Singlet-A 1.9925 eV 622.24 nm f=0.0000 <S**2>=0.000
244 ->252 -0.43563
248 ->252 0.54973

Excited State 29: Singlet-E 1.9930 eV 622.10 nm f=0.0049 <S**2>=0.000
242 ->252 -0.11475
243 ->252 -0.10362
246 ->252 0.40528
247 ->252 0.54317

Excited State 30: Singlet-E 1.9930 eV 622.10 nm f=0.0049 <S**2>=0.000
242 ->252 -0.10362
243 ->252 0.11477
246 ->252 0.54317

247 ->252 -0.40528

Excited State 31: Singlet-B 1.9945 eV 621.64 nm f=0.0032 <S**2>=0.000
245 ->252 0.65472
249 ->252 -0.24023

Excited State 32: Singlet-A 2.0273 eV 611.57 nm f=0.0000 <S**2>=0.000
234 ->250 0.15817
235 ->251 0.15818
244 ->252 0.52533
248 ->252 0.38675

Excited State 33: Singlet-E 2.0426 eV 607.00 nm f=0.0827 <S**2>=0.000
236 ->250 0.41743
236 ->251 -0.26149
237 ->250 -0.22102
242 ->252 -0.38547
243 ->252 -0.19085

Excited State 34: Singlet-E 2.0426 eV 607.00 nm f=0.0827 <S**2>=0.000
236 ->250 0.26150
236 ->251 0.41744
237 ->251 0.22102
242 ->252 0.19085
243 ->252 -0.38546

Excited State 35: Singlet-E 2.0752 eV 597.45 nm f=0.0640 <S**2>=0.000
236 ->251 0.45358
242 ->252 -0.36501
243 ->252 0.33109
246 ->252 -0.13829

Excited State 36: Singlet-E 2.0752 eV 597.45 nm f=0.0640 <S**2>=0.000
236 ->250 0.45358
242 ->252 0.33108
243 ->252 0.36501
247 ->252 0.13829

Excited state symmetry could not be determined.
Excited State 37: Singlet-?Sym 2.1061 eV 588.69 nm f=0.0047 <S**2>=0.000
234 ->250 0.26791
234 ->251 0.41792
235 ->250 0.41794
235 ->251 -0.26788

Excited state symmetry could not be determined.
Excited State 38: Singlet-?Sym 2.1098 eV 587.65 nm f=0.0000 <S**2>=0.000
234 ->251 0.48792
235 ->250 -0.48790

Excited state symmetry could not be determined.
Excited State 39: Singlet-?Sym 2.1425 eV 578.68 nm f=0.0233 <S**2>=0.000
234 ->250 0.39667
234 ->251 -0.26842
235 ->250 -0.26844
235 ->251 -0.39661
249 ->252 0.17123

Excited State 40: Singlet-E 2.1576 eV 574.64 nm f=0.0001 <S**2>=0.000
233 ->251 0.70520

Excited State 41: Singlet-E 2.1576 eV 574.64 nm f=0.0001 <S**2>=0.000
233 ->250 0.70520

Excited state symmetry could not be determined.
Excited State 42: Singlet-?Sym 2.1888 eV 566.44 nm f=0.0000 <S**2>=0.000
234 ->250 0.45835
235 ->251 0.45841
244 ->252 -0.14300
248 ->252 -0.17648

Excited State 43: Singlet-B 2.4045 eV 515.63 nm f=0.0036 <S**2>=0.000
241 ->252 0.69985

Excited State 44: Singlet-E 2.4106 eV 514.33 nm f=0.0072 <S**2>=0.000
239 ->252 0.69570

Excited State 45: Singlet-E 2.4106 eV 514.33 nm f=0.0072 <S**2>=0.000
238 ->252 0.69570

Excited State 46: Singlet-A 2.4129 eV 513.85 nm f=0.0000 <S**2>=0.000
240 ->252 0.69945

Excited State 47: Singlet-E 2.5098 eV 494.01 nm f=0.0375 <S**2>=0.000
225 ->251 -0.10724
229 ->250 0.28577
229 ->251 -0.12473
232 ->250 0.24674
232 ->251 0.53136
237 ->251 -0.10411

Excited State 48: Singlet-E 2.5098 eV 494.01 nm f=0.0375 <S**2>=0.000
225 ->250 -0.10725
229 ->250 -0.12473
229 ->251 -0.28577
232 ->250 0.53135
232 ->251 -0.24675
237 ->250 -0.10411

Excited state symmetry could not be determined.
Excited State 49: Singlet-?Sym 2.5240 eV 491.21 nm f=0.0000 <S**2>=0.000
230 ->251 -0.49168
231 ->250 0.49169

Excited state symmetry could not be determined.
Excited State 50: Singlet-?Sym 2.5331 eV 489.46 nm f=0.0001 <S**2>=0.000
230 ->250 -0.16542
230 ->251 0.47156
231 ->250 0.47155
231 ->251 0.16542

Excited State 51: Singlet-A 2.5581 eV 484.68 nm f=0.0000 <S**2>=0.000
242 ->254 0.10118
243 ->255 -0.10118
244 ->256 -0.14454
245 ->257 -0.18141
246 ->258 -0.15688
247 ->259 -0.15688
248 ->256 0.10696
249 ->253 0.58332

Excited State 52: Singlet-E 2.5703 eV 482.38 nm f=0.0008 <S**2>=0.000
244 ->258 -0.15340
245 ->255 -0.19733
245 ->258 -0.12551
246 ->253 0.13710
246 ->256 -0.10779
246 ->257 -0.14676
247 ->253 0.23146
248 ->259 0.13356
249 ->254 0.40460
249 ->255 0.11677
249 ->259 0.16759

Excited State 53: Singlet-E 2.5703 eV 482.38 nm f=0.0008 <S**2>=0.000

244 ->259 -0.15340
245 ->254 0.19732
245 ->259 0.12552
246 ->253 0.23144
247 ->253 -0.13711
247 ->256 -0.10777
247 ->257 0.14678
248 ->258 -0.13355
249 ->254 -0.11677
249 ->255 0.40461
249 ->258 0.16757

Excited State 54: Singlet-B 2.5746 eV 481.56 nm f=0.0000 <S**2>=0.000
242 ->258 0.14974
243 ->259 -0.14976
244 ->253 0.24064
244 ->257 -0.13642
246 ->254 0.24150
247 ->255 0.24153
248 ->253 -0.29195
248 ->257 -0.14031
249 ->256 0.36707

Excited State 55: Singlet-A 2.5755 eV 481.40 nm f=0.0000 <S**2>=0.000
242 ->258 0.12786
243 ->259 0.12784
244 ->256 -0.11588
245 ->253 0.38491
246 ->254 0.20468
247 ->255 -0.20465
248 ->256 -0.16753
249 ->257 0.37023

Excited State 56: Singlet-E 2.5770 eV 481.11 nm f=0.0003 <S**2>=0.000
242 ->253 -0.16049
243 ->253 -0.11214
243 ->257 0.12765
244 ->255 0.19893
245 ->255 -0.15542
245 ->258 0.16024
246 ->256 0.15130
247 ->253 0.23325
248 ->254 0.17234
248 ->255 -0.11061
248 ->259 0.12181

249 ->254 -0.22783
249 ->259 0.31417

Excited State 57: Singlet-E 2.5770 eV 481.11 nm f=0.0003 <S**2>=0.000
242 ->253 -0.11214
242 ->257 0.12764
243 ->253 0.16049
244 ->254 0.19894
245 ->254 0.15542
245 ->259 -0.16024
246 ->253 0.23326
247 ->256 0.15128
248 ->254 -0.11061
248 ->255 -0.17234
248 ->258 -0.12181
249 ->255 -0.22781
249 ->258 0.31418

Excited State 58: Singlet-B 2.5884 eV 479.00 nm f=0.0000 <S**2>=0.000
242 ->254 -0.17625
243 ->255 -0.17625
244 ->253 0.30427
244 ->257 0.14877
245 ->256 0.21382
246 ->255 0.12334
246 ->258 0.18762
247 ->254 -0.12333
247 ->259 -0.18762
248 ->253 0.34141
248 ->257 -0.15403

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 2.6101 eV 475.02 nm f=0.0012 <S**2>=0.000
226 ->250 0.21427
226 ->251 0.12977
227 ->250 0.12986
227 ->251 -0.21459
230 ->250 -0.40617
230 ->251 -0.13784
231 ->250 -0.13795
231 ->251 0.40678

Excited state symmetry could not be determined.
Excited State 60: Singlet-?Sym 2.6108 eV 474.89 nm f=0.0000 <S**2>=0.000
226 ->250 -0.23578

227 ->251 -0.23548
230 ->250 0.42976
231 ->251 0.42918

Excited State 61: Singlet-E 2.6304 eV 471.35 nm f=0.0050 <S**2>=0.000
242 ->253 -0.30261
244 ->254 0.15536
246 ->253 -0.19931
247 ->253 -0.23372
248 ->254 0.22036
249 ->254 0.42946

Excited State 62: Singlet-E 2.6304 eV 471.35 nm f=0.0050 <S**2>=0.000
243 ->253 0.30261
244 ->255 -0.15535
246 ->253 -0.23372
247 ->253 0.19932
248 ->255 -0.22035
249 ->255 0.42946

Excited State 63: Singlet-E 2.6384 eV 469.92 nm f=0.0053 <S**2>=0.000
228 ->250 0.69372

Excited State 64: Singlet-E 2.6384 eV 469.92 nm f=0.0053 <S**2>=0.000
228 ->251 0.69372

Excited State 65: Singlet-A 2.6387 eV 469.87 nm f=0.0000 <S**2>=0.000
242 ->254 -0.19139
243 ->255 0.19139
245 ->253 0.31999
245 ->257 0.10985
246 ->254 -0.28986
247 ->255 0.28986
249 ->253 0.25586

Excited State 66: Singlet-B 2.6426 eV 469.18 nm f=0.0003 <S**2>=0.000
244 ->253 -0.21439
246 ->254 0.31815
247 ->255 0.31816
248 ->253 0.46287

Excited State 67: Singlet-E 2.6448 eV 468.79 nm f=0.0004 <S**2>=0.000
242 ->253 -0.11145
245 ->255 0.23624
246 ->253 0.11332

247 ->253 0.43274
248 ->254 0.24759
248 ->255 0.34713
249 ->259 -0.14380

Excited State 68: Singlet-E 2.6448 eV 468.79 nm f=0.0004 <S**2>=0.000
243 ->253 0.11146
245 ->254 -0.23624
246 ->253 0.43274
247 ->253 -0.11331
248 ->254 0.34712
248 ->255 -0.24759
249 ->258 -0.14380

Excited state symmetry could not be determined.
Excited State 69: Singlet-?Sym 2.6468 eV 468.44 nm f=0.0000 <S**2>=0.000
226 ->251 -0.45939
227 ->250 0.45945
245 ->253 -0.19479

Excited state symmetry could not be determined.
Excited State 70: Singlet-?Sym 2.6494 eV 467.97 nm f=0.0005 <S**2>=0.000
226 ->250 -0.17698
226 ->251 0.46237
227 ->250 0.46230
227 ->251 0.17697

Excited State 71: Singlet-A 2.6514 eV 467.61 nm f=0.0000 <S**2>=0.000
226 ->251 -0.15920
227 ->250 0.15922
242 ->254 0.26159
243 ->255 -0.26159
245 ->253 0.36650
245 ->257 -0.10132
246 ->254 -0.10384
246 ->255 0.17960
247 ->254 0.17962
247 ->255 0.10382
249 ->253 -0.17750
249 ->257 -0.12252

Excited State 72: Singlet-E 2.6560 eV 466.82 nm f=0.0125 <S**2>=0.000
225 ->250 -0.20113
225 ->251 0.55100
229 ->251 0.29587

232 ->250 0.10043

Excited State 73: Singlet-E 2.6560 eV 466.82 nm f=0.0125 <S**2>=0.000
225 ->250 0.55100
225 ->251 0.20113
229 ->250 0.29587
232 ->251 -0.10043

Excited State 74: Singlet-B 2.6581 eV 466.44 nm f=0.0004 <S**2>=0.000
242 ->254 0.17870
243 ->255 0.17873
244 ->253 0.40382
246 ->255 -0.35560
247 ->254 0.35561
248 ->253 0.10585

Excited State 75: Singlet-E 2.6605 eV 466.02 nm f=0.0009 <S**2>=0.000
225 ->251 0.13454
242 ->253 0.38573
243 ->253 0.17420
245 ->254 0.30763
245 ->255 -0.21314
248 ->254 0.33391

Excited State 76: Singlet-E 2.6605 eV 466.02 nm f=0.0009 <S**2>=0.000
225 ->250 -0.13455
242 ->253 -0.17419
243 ->253 0.38573
245 ->254 -0.21314
245 ->255 -0.30762
248 ->255 0.33390

Excited State 77: Singlet-B 2.6637 eV 465.45 nm f=0.0000 <S**2>=0.000
242 ->258 -0.13724
243 ->259 0.13723
244 ->253 -0.16810
244 ->257 0.15545
246 ->254 -0.10675
246 ->255 -0.15088
247 ->254 0.15091
247 ->255 -0.10675
248 ->257 0.21326
249 ->256 0.48893

Excited state symmetry could not be determined.

Excited State 78: Singlet-?Sym 2.6656 eV 465.13 nm f=0.0000 <S**2>=0.000
242 ->254 -0.20353
243 ->255 0.20348
246 ->255 0.40530
247 ->254 0.40531
248 ->256 -0.10257
249 ->257 -0.20312

Excited State 79: Singlet-E 2.6671 eV 464.87 nm f=0.0000 <S**2>=0.000
242 ->256 -0.12429
242 ->257 -0.12394
244 ->255 0.24827
244 ->258 0.10300
245 ->254 -0.17252
245 ->255 0.20518
246 ->257 -0.10328
248 ->258 0.25123
249 ->258 0.46051

Excited State 80: Singlet-E 2.6671 eV 464.87 nm f=0.0000 <S**2>=0.000
243 ->256 0.12426
243 ->257 -0.12395
244 ->254 -0.24834
244 ->259 -0.10299
245 ->254 0.20520
245 ->255 0.17251
247 ->257 -0.10330
248 ->259 -0.25122
249 ->259 0.46048

Excited State 81: Singlet-A 2.6671 eV 464.87 nm f=0.0000 <S**2>=0.000
242 ->258 -0.13090
243 ->259 -0.13092
244 ->256 0.13854
246 ->255 0.19030
247 ->254 0.19027
248 ->256 0.29808
249 ->257 0.46974

Excited state symmetry could not be determined.
Excited State 82: Singlet-?Sym 2.6696 eV 464.43 nm f=0.0004 <S**2>=0.000
242 ->254 0.28108
243 ->255 0.28110
244 ->253 0.20686
246 ->255 0.28346

246 ->258 -0.10664
247 ->254 -0.28343
247 ->259 0.10665
248 ->257 0.20664
249 ->256 0.19500

Excited State 83: Singlet-E 2.6708 eV 464.22 nm f=0.0000 <S**2>=0.000
242 ->253 0.26327
244 ->254 0.49614
244 ->259 -0.11749
245 ->254 -0.25197
248 ->259 -0.11696
249 ->259 0.19651

Excited State 84: Singlet-E 2.6708 eV 464.22 nm f=0.0000 <S**2>=0.000
243 ->253 0.26325
244 ->255 0.49619
244 ->258 -0.11748
245 ->255 0.25199
248 ->258 -0.11692
249 ->258 -0.19645

Excited state symmetry could not be determined.
Excited State 85: Singlet-?Sym 2.6749 eV 463.51 nm f=0.0004 <S**2>=0.000
226 ->250 -0.41176
226 ->251 -0.12745
227 ->250 -0.12747
227 ->251 0.41212
230 ->250 -0.22409
231 ->251 0.22428

Excited state symmetry could not be determined.
Excited State 86: Singlet-?Sym 2.6757 eV 463.37 nm f=0.0000 <S**2>=0.000
226 ->250 0.43367
227 ->251 0.43333
230 ->250 0.23093
231 ->251 0.23073

Excited state symmetry could not be determined.
Excited State 87: Singlet-?Sym 2.6905 eV 460.82 nm f=0.0000 <S**2>=0.000
242 ->255 0.47211
243 ->254 0.47425
248 ->256 0.15250

Excited state symmetry could not be determined.

Excited State 88: Singlet-?Sym 2.6906 eV 460.80 nm f=0.0000 <S**2>=0.000
242 ->255 0.46786
243 ->254 -0.46569
245 ->256 0.10072
248 ->257 0.18774

Excited State 89: Singlet-E 2.6987 eV 459.43 nm f=0.0000 <S**2>=0.000
246 ->256 0.23701
246 ->257 0.17514
247 ->256 0.40001
248 ->258 0.40923
248 ->259 0.22099

Excited State 90: Singlet-E 2.6987 eV 459.43 nm f=0.0000 <S**2>=0.000
246 ->256 -0.39997
247 ->256 0.23701
247 ->257 -0.17519
248 ->258 -0.22101
248 ->259 0.40924

Excited State 91: Singlet-A 2.6992 eV 459.33 nm f=0.0000 <S**2>=0.000
244 ->256 -0.17301
246 ->258 0.28900
246 ->259 -0.16591
247 ->258 0.16599
247 ->259 0.28897
248 ->256 0.45616

Excited State 92: Singlet-B 2.7001 eV 459.18 nm f=0.0000 <S**2>=0.000
244 ->257 -0.11538
246 ->258 0.26968
246 ->259 0.22150
247 ->258 0.22152
247 ->259 -0.26975
248 ->257 0.46206

Excited State 93: Singlet-B 2.7020 eV 458.86 nm f=0.0000 <S**2>=0.000
245 ->256 0.46789
246 ->258 -0.22427
246 ->259 0.29096
247 ->258 0.29113
247 ->259 0.22416

Excited State 94: Singlet-E 2.7020 eV 458.85 nm f=0.0000 <S**2>=0.000
245 ->258 0.21679

246 ->256 -0.17499
246 ->257 -0.15748
247 ->256 0.28208
247 ->257 0.51137
248 ->259 -0.16614

Excited State 95: Singlet-E 2.7020 eV 458.85 nm f=0.0000 <S**2>=0.000
245 ->259 -0.21681
246 ->256 -0.28204
246 ->257 0.51142
247 ->256 -0.17495
247 ->257 0.15749
248 ->258 0.16611

Excited state symmetry could not be determined.
Excited State 96: Singlet-?Sym 2.7030 eV 458.70 nm f=0.0000 <S**2>=0.000
245 ->257 -0.18389
246 ->258 0.15340
246 ->259 0.44434
247 ->258 -0.44423
247 ->259 0.15345

Excited State 97: Singlet-A 2.7051 eV 458.33 nm f=0.0000 <S**2>=0.000
244 ->256 -0.28968
245 ->257 0.57041
246 ->258 -0.12353
246 ->259 0.11226
247 ->258 -0.11297
247 ->259 -0.12356
248 ->256 0.12577

Excited State 98: Singlet-B 2.7055 eV 458.27 nm f=0.0000 <S**2>=0.000
242 ->258 0.11547
243 ->259 -0.11568
244 ->257 -0.34515
245 ->256 0.36936
246 ->259 -0.30317
247 ->258 -0.30287
248 ->257 0.16740

Excited State 99: Singlet-E 2.7060 eV 458.19 nm f=0.0000 <S**2>=0.000
242 ->256 0.11563
242 ->257 0.10889
244 ->258 -0.27766
245 ->258 0.55370

246 ->257 -0.10211
247 ->256 -0.14818
247 ->257 -0.10949
248 ->258 0.16671

Excited State 100: Singlet-E 2.7060 eV 458.19 nm f=0.0000 <S**2>=0.000
243 ->256 -0.11563
243 ->257 0.10892
244 ->259 0.27769
245 ->259 0.55369
246 ->256 -0.14818
246 ->257 0.10953
247 ->257 -0.10210
248 ->259 -0.16671

Table S4: Vertical Excitation energies of $TAP^{FcCN}Mg$ using BP86 PCM-TDDFT

Excited State 1: Singlet-E 0.6412 eV 1933.53 nm f=0.0004 <S**2>=0.000
269 ->274 -0.23426
269 ->275 0.23174
272 ->274 0.39594
272 ->275 0.43592
273 ->275 0.20175
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3459.82586563
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-E 0.6412 eV 1933.53 nm f=0.0004 <S**2>=0.000
269 ->274 0.23174
269 ->275 0.23426
272 ->274 -0.43592
272 ->275 0.39594
273 ->274 -0.20175

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 0.6436 eV 1926.37 nm f=0.0000 <S**2>=0.000
270 ->274 -0.48340
270 ->275 0.12708
271 ->274 0.12710
271 ->275 0.48340

Excited State 4: Singlet-E 0.6474 eV 1915.05 nm f=0.0002 <S**2>=0.000
269 ->274 -0.59489
269 ->275 0.16569

272 ->274 -0.31899
272 ->275 -0.11551

Excited State 5: Singlet-E 0.6474 eV 1915.05 nm f=0.0002 <S**2>=0.000
269 ->274 0.16570
269 ->275 0.59489
272 ->274 0.11551
272 ->275 -0.31899

Excited state symmetry could not be determined.
Excited State 6: Singlet-?Sym 0.6478 eV 1913.90 nm f=0.0000 <S**2>=0.000
270 ->274 0.12738
270 ->275 0.48251
271 ->274 0.48257
271 ->275 -0.12738

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 0.6482 eV 1912.86 nm f=0.0000 <S**2>=0.000
270 ->275 0.49916
271 ->274 -0.49909

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 0.6496 eV 1908.54 nm f=0.0002 <S**2>=0.000
270 ->274 0.48862
271 ->275 0.48862

Excited State 9: Singlet-E 0.6706 eV 1848.80 nm f=0.0084 <S**2>=0.000
268 ->274 -0.47711
268 ->275 -0.10355
272 ->274 -0.10343
272 ->275 0.14029
273 ->274 0.47543

Excited State 10: Singlet-E 0.6706 eV 1848.80 nm f=0.0084 <S**2>=0.000
268 ->274 -0.10355
268 ->275 0.47711
272 ->274 -0.14029
272 ->275 -0.10343
273 ->275 0.47543

Excited state symmetry could not be determined.
Excited State 11: Singlet-?Sym 0.7191 eV 1724.11 nm f=0.0000 <S**2>=0.000
266 ->274 0.49972
267 ->275 -0.49971

Excited state symmetry could not be determined.
Excited State 12: Singlet-?Sym 0.7326 eV 1692.30 nm f=0.0000 <S**2>=0.000
266 ->274 0.48800
266 ->275 0.10571
267 ->274 -0.10571
267 ->275 0.48801

Excited state symmetry could not be determined.
Excited State 13: Singlet-?Sym 0.8940 eV 1386.91 nm f=0.0180 <S**2>=0.000
262 ->274 0.11147
263 ->275 0.11147
266 ->275 -0.46211
267 ->274 0.46211
273 ->276 -0.11277

Excited State 14: Singlet-E 0.9014 eV 1375.39 nm f=0.1572 <S**2>=0.000
264 ->275 0.12442
265 ->275 -0.15581
268 ->274 0.20091
268 ->275 0.44180
273 ->274 0.26089
273 ->275 -0.36348

Excited State 15: Singlet-E 0.9014 eV 1375.39 nm f=0.1572 <S**2>=0.000
264 ->274 0.12442
265 ->274 0.15581
268 ->274 0.44180
268 ->275 -0.20091
273 ->274 0.36348
273 ->275 0.26089

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 0.9398 eV 1319.27 nm f=0.0000 <S**2>=0.000
262 ->274 0.18225
263 ->275 -0.18225
266 ->275 0.45973
267 ->274 0.45973
268 ->276 -0.10459

Excited State 17: Singlet-E 1.0389 eV 1193.41 nm f=0.0050 <S**2>=0.000
264 ->274 -0.23958
264 ->275 0.40869
265 ->274 0.22928
265 ->275 0.46829

Excited State 18: Singlet-E 1.0389 eV 1193.41 nm f=0.0050 <S**2>=0.000
264 ->274 -0.40869
264 ->275 -0.23958
265 ->274 0.46829
265 ->275 -0.22928

Excited state symmetry could not be determined.
Excited State 19: Singlet-?Sym 1.0502 eV 1180.63 nm f=0.0000 <S**2>=0.000
262 ->274 -0.10771
262 ->275 0.48813
263 ->274 0.48816
263 ->275 0.10771

Excited state symmetry could not be determined.
Excited State 20: Singlet-?Sym 1.0527 eV 1177.79 nm f=0.0000 <S**2>=0.000
262 ->275 0.49669
263 ->274 -0.49667

Excited State 21: Singlet-E 1.1224 eV 1104.63 nm f=0.0945 <S**2>=0.000
264 ->274 0.44264
264 ->275 -0.23933
265 ->274 0.36487
265 ->275 0.24211
268 ->274 -0.12450
273 ->274 -0.13007

Excited State 22: Singlet-E 1.1224 eV 1104.63 nm f=0.0945 <S**2>=0.000
264 ->274 0.23933
264 ->275 0.44264
265 ->274 0.24211
265 ->275 -0.36487
268 ->275 -0.12450
273 ->275 0.13007

Excited state symmetry could not be determined.
Excited State 23: Singlet-?Sym 1.1238 eV 1103.24 nm f=0.0080 <S**2>=0.000
262 ->274 0.48109
263 ->275 0.48109

Excited state symmetry could not be determined.
Excited State 24: Singlet-?Sym 1.1487 eV 1079.35 nm f=0.0000 <S**2>=0.000
262 ->274 0.44933
262 ->275 0.10198
263 ->274 0.10198
263 ->275 -0.44933

266 ->275 -0.17329
267 ->274 -0.17329
268 ->276 0.10910

Excited State 25: Singlet-B 1.5153 eV 818.20 nm f=0.0001 <S**2>=0.000
272 ->276 0.69808
273 ->276 0.10724

Excited State 26: Singlet-E 1.5178 eV 816.85 nm f=0.0020 <S**2>=0.000
270 ->276 0.59294
271 ->276 -0.38023

Excited State 27: Singlet-E 1.5178 eV 816.85 nm f=0.0020 <S**2>=0.000
270 ->276 0.38023
271 ->276 0.59294

Excited State 28: Singlet-A 1.5180 eV 816.76 nm f=0.0000 <S**2>=0.000
269 ->276 0.70405

Excited State 29: Singlet-B 1.5856 eV 781.95 nm f=0.0317 <S**2>=0.000
272 ->276 -0.10561
273 ->276 0.67238

Excited State 30: Singlet-A 1.6357 eV 757.98 nm f=0.0000 <S**2>=0.000
268 ->276 0.67674

Excited State 31: Singlet-E 1.6464 eV 753.05 nm f=0.0373 <S**2>=0.000
261 ->274 -0.14605
267 ->276 0.67055

Excited State 32: Singlet-E 1.6464 eV 753.05 nm f=0.0373 <S**2>=0.000
261 ->275 0.14606
266 ->276 0.67054

Excited State 33: Singlet-E 1.7860 eV 694.19 nm f=0.1917 <S**2>=0.000
256 ->275 -0.15738
260 ->274 0.10050
260 ->275 0.12313
261 ->274 0.39970
261 ->275 -0.48920
266 ->276 0.12321

Excited State 34: Singlet-E 1.7860 eV 694.19 nm f=0.1917 <S**2>=0.000
256 ->274 0.15738
260 ->274 0.12313

260 ->275 -0.10050
261 ->274 0.48920
261 ->275 0.39970
267 ->276 0.12321

Excited State 35: Singlet-E 1.8986 eV 653.02 nm f=0.0876 <S**2>=0.000
260 ->274 -0.34259
260 ->275 0.53380
261 ->275 0.13976
262 ->276 -0.14668
263 ->276 -0.19678

Excited State 36: Singlet-E 1.8986 eV 653.02 nm f=0.0876 <S**2>=0.000
260 ->274 0.53380
260 ->275 0.34259
261 ->274 -0.13976
262 ->276 0.19678
263 ->276 -0.14668

Excited State 37: Singlet-B 1.9032 eV 651.44 nm f=0.0000 <S**2>=0.000
258 ->274 0.13266
258 ->275 -0.19654
259 ->274 0.19654
259 ->275 0.13266
265 ->276 0.62103

Excited State 38: Singlet-A 1.9184 eV 646.30 nm f=0.0000 <S**2>=0.000
258 ->274 0.16139
258 ->275 0.18414
259 ->274 0.18414
259 ->275 -0.16140
264 ->276 0.61497

Excited state symmetry could not be determined.
Excited State 39: Singlet-?Sym 1.9230 eV 644.74 nm f=0.0045 <S**2>=0.000
258 ->274 0.45776
259 ->275 0.45775
265 ->276 -0.24880

Excited state symmetry could not be determined.
Excited State 40: Singlet-?Sym 1.9325 eV 641.58 nm f=0.0000 <S**2>=0.000
258 ->274 0.46908
259 ->275 -0.46909
264 ->276 -0.23506

Excited State 41: Singlet-E 1.9399 eV 639.13 nm f=0.0238 <S**2>=0.000
260 ->274 -0.20284
260 ->275 0.13025
262 ->276 0.57702
263 ->276 0.31154

Excited State 42: Singlet-E 1.9399 eV 639.13 nm f=0.0239 <S**2>=0.000
260 ->274 0.13025
260 ->275 0.20284
262 ->276 -0.31154
263 ->276 0.57702

Excited state symmetry could not be determined.
Excited State 43: Singlet-?Sym 1.9939 eV 621.82 nm f=0.0301 <S**2>=0.000
258 ->274 -0.14641
258 ->275 -0.43875
259 ->274 0.43877
259 ->275 -0.14641
265 ->276 -0.21185

Excited state symmetry could not be determined.
Excited State 44: Singlet-?Sym 2.0097 eV 616.93 nm f=0.0000 <S**2>=0.000
258 ->275 0.44710
259 ->274 0.44708
260 ->276 -0.10900
264 ->276 -0.24506
268 ->276 0.10308

Excited State 45: Singlet-E 2.0237 eV 612.66 nm f=0.0003 <S**2>=0.000
257 ->275 0.70253

Excited State 46: Singlet-E 2.0237 eV 612.66 nm f=0.0003 <S**2>=0.000
257 ->274 0.70253

Excited State 47: Singlet-E 2.2770 eV 544.50 nm f=0.0311 <S**2>=0.000
249 ->275 -0.11520
252 ->275 0.16915
253 ->274 -0.13223
253 ->275 0.49311
256 ->275 -0.42826

Excited State 48: Singlet-E 2.2770 eV 544.50 nm f=0.0311 <S**2>=0.000
249 ->274 -0.11520
252 ->274 -0.16915
253 ->274 0.49311

253 ->275 0.13223
256 ->274 -0.42826

Excited state symmetry could not be determined.
Excited State 49: Singlet-?Sym 2.2857 eV 542.43 nm f=0.0009 <S**2>=0.000
254 ->274 0.49905
255 ->275 0.49909

Excited state symmetry could not be determined.
Excited State 50: Singlet-?Sym 2.2858 eV 542.40 nm f=0.0000 <S**2>=0.000
254 ->274 0.47651
254 ->275 0.14882
255 ->274 0.14883
255 ->275 -0.47647

Excited State 51: Singlet-E 2.2937 eV 540.54 nm f=0.0010 <S**2>=0.000
252 ->274 0.29523
252 ->275 0.61945
256 ->275 0.11098

Excited State 52: Singlet-E 2.2937 eV 540.54 nm f=0.0010 <S**2>=0.000
252 ->274 0.61945
252 ->275 -0.29523
256 ->274 -0.11097

Excited state symmetry could not be determined.
Excited State 53: Singlet-?Sym 2.2958 eV 540.05 nm f=0.0000 <S**2>=0.000
254 ->275 0.49892
255 ->274 -0.49876

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 2.2960 eV 540.00 nm f=0.0000 <S**2>=0.000
254 ->274 -0.14779
254 ->275 0.47621
255 ->274 0.47638
255 ->275 0.14779

Excited State 55: Singlet-E 2.3810 eV 520.73 nm f=0.0716 <S**2>=0.000
249 ->274 -0.16657
249 ->275 -0.21383
253 ->274 0.40186
253 ->275 -0.16557
256 ->274 0.35149
256 ->275 -0.28716

Excited State 56: Singlet-E 2.3810 eV 520.73 nm f=0.0716 <S**2>=0.000
249 ->274 0.21385
249 ->275 -0.16659
253 ->274 0.16557
253 ->275 0.40186
256 ->274 0.28716
256 ->275 0.35148

Excited state symmetry could not be determined.
Excited State 57: Singlet-?Sym 2.4348 eV 509.21 nm f=0.0000 <S**2>=0.000
250 ->274 -0.31882
250 ->275 -0.38509
251 ->274 0.38507
251 ->275 -0.31878

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 2.4419 eV 507.73 nm f=0.0000 <S**2>=0.000
250 ->274 -0.45993
250 ->275 -0.19566
251 ->274 -0.19569
251 ->275 0.45996

Excited State 59: Singlet-A 2.5199 eV 492.02 nm f=0.0000 <S**2>=0.000
269 ->280 -0.10918
270 ->282 -0.10606
271 ->283 -0.10606
272 ->281 -0.11259
273 ->277 0.65677

Excited state symmetry could not be determined.
Excited State 60: Singlet-?Sym 2.5209 eV 491.82 nm f=0.0003 <S**2>=0.000
250 ->274 -0.19164
250 ->275 0.44833
251 ->274 0.44832
251 ->275 0.19164
257 ->276 -0.12373

Excited state symmetry could not be determined.
Excited State 61: Singlet-?Sym 2.5232 eV 491.38 nm f=0.0000 <S**2>=0.000
250 ->274 0.37916
250 ->275 -0.31323
251 ->274 0.31324
251 ->275 0.37916

Excited State 62: Singlet-A 2.5377 eV 488.56 nm f=0.0000 <S**2>=0.000

272 ->277 0.67106
273 ->281 0.13010

Excited State 63: Singlet-E 2.5383 eV 488.45 nm f=0.0001 <S**2>=0.000
270 ->277 0.66801
273 ->282 0.12305

Excited State 64: Singlet-E 2.5383 eV 488.45 nm f=0.0001 <S**2>=0.000
271 ->277 0.66801
273 ->283 0.12305

Excited State 65: Singlet-B 2.5392 eV 488.27 nm f=0.0000 <S**2>=0.000
269 ->277 0.67461
273 ->280 0.13152

Excited State 66: Singlet-E 2.5653 eV 483.30 nm f=0.0026 <S**2>=0.000
269 ->283 -0.11902
271 ->280 -0.10606
271 ->281 -0.13188
272 ->279 -0.13222
272 ->283 -0.12726
273 ->278 0.58640
273 ->279 -0.19292

Excited State 67: Singlet-E 2.5653 eV 483.30 nm f=0.0026 <S**2>=0.000
269 ->282 -0.11902
270 ->280 -0.10605
270 ->281 0.13188
272 ->278 0.13222
272 ->282 0.12727
273 ->278 0.19292
273 ->279 0.58640

Excited State 68: Singlet-B 2.5739 eV 481.70 nm f=0.0048 <S**2>=0.000
261 ->276 0.15351
268 ->277 0.59858
269 ->281 -0.13829
270 ->279 -0.10532
270 ->282 0.12720
271 ->278 -0.10532
271 ->283 -0.12720
272 ->280 -0.13807

Excited State 69: Singlet-B 2.5856 eV 479.52 nm f=0.0522 <S**2>=0.000
261 ->276 0.64378

268 ->277 -0.20317

Excited State 70: Singlet-E 2.5888 eV 478.92 nm f=0.0003 <S**2>=0.000
267 ->281 0.10448
268 ->283 0.11540
269 ->278 0.22675
269 ->279 -0.38643
272 ->278 0.42493
273 ->283 0.19477

Excited State 71: Singlet-E 2.5888 eV 478.92 nm f=0.0003 <S**2>=0.000
266 ->281 -0.10448
268 ->282 0.11539
269 ->278 -0.38644
269 ->279 -0.22675
272 ->279 0.42494
273 ->282 -0.19476

Excited state symmetry could not be determined.
Excited State 72: Singlet-?Sym 2.5889 eV 478.91 nm f=0.0001 <S**2>=0.000
266 ->282 0.10345
267 ->283 -0.10345
268 ->281 -0.13210
270 ->278 -0.36876
270 ->279 -0.25714
271 ->278 -0.25715
271 ->279 0.36877
273 ->280 -0.20882

Excited state symmetry could not be determined.
Excited State 73: Singlet-?Sym 2.5909 eV 478.54 nm f=0.0000 <S**2>=0.000
266 ->282 -0.10898
267 ->283 -0.10898
268 ->280 -0.13849
270 ->278 0.16731
270 ->279 0.41376
271 ->278 -0.41375
271 ->279 0.16730
273 ->281 -0.21735

Excited State 74: Singlet-E 2.5972 eV 477.37 nm f=0.0041 <S**2>=0.000
266 ->277 0.12541
269 ->278 0.40163
269 ->279 -0.23849
272 ->278 -0.39859

272 ->279 0.27628
273 ->279 0.14357

Excited State 75: Singlet-E 2.5972 eV 477.37 nm f=0.0041 <S**2>=0.000
267 ->277 -0.12541
269 ->278 0.23849
269 ->279 0.40163
272 ->278 0.27628
272 ->279 0.39859
273 ->278 0.14357

Excited state symmetry could not be determined.
Excited State 76: Singlet-?Sym 2.5978 eV 477.26 nm f=0.0041 <S**2>=0.000
261 ->276 0.13190
268 ->277 0.15523
270 ->278 -0.27306
270 ->279 0.39149
271 ->278 0.39149
271 ->279 0.27305

Excited state symmetry could not be determined.
Excited State 77: Singlet-?Sym 2.5996 eV 476.94 nm f=0.0000 <S**2>=0.000
270 ->278 0.45999
270 ->279 -0.18497
271 ->278 0.18497
271 ->279 0.45999

Excited State 78: Singlet-E 2.6083 eV 475.34 nm f=0.0126 <S**2>=0.000
267 ->277 0.59988
269 ->279 0.15486
269 ->283 -0.10894
271 ->280 -0.10816
271 ->281 -0.10238
272 ->278 0.10393
272 ->283 -0.10850
273 ->278 -0.13243
273 ->279 0.11260

Excited State 79: Singlet-E 2.6083 eV 475.34 nm f=0.0126 <S**2>=0.000
266 ->277 0.59988
269 ->278 -0.15486
269 ->282 0.10894
270 ->280 0.10815
270 ->281 -0.10239
272 ->279 -0.10392

272 ->282 -0.10850
273 ->278 0.11260
273 ->279 0.13243

Excited State 80: Singlet-E 2.6312 eV 471.21 nm f=0.0016 <S**2>=0.000
266 ->277 -0.20995
268 ->278 0.46002
268 ->279 0.44476

Excited State 81: Singlet-E 2.6312 eV 471.21 nm f=0.0017 <S**2>=0.000
267 ->277 -0.20995
268 ->278 0.44476
268 ->279 -0.46002

Excited state symmetry could not be determined.
Excited State 82: Singlet-?Sym 2.6460 eV 468.57 nm f=0.0000 <S**2>=0.000
266 ->278 -0.13922
266 ->279 -0.40139
267 ->278 0.40139
267 ->279 -0.13922
269 ->280 -0.16421
270 ->282 -0.15894
271 ->283 -0.15894
272 ->281 -0.16421
273 ->277 -0.13623

Excited state symmetry could not be determined.
Excited State 83: Singlet-?Sym 2.6476 eV 468.28 nm f=0.0093 <S**2>=0.000
261 ->276 -0.11699
266 ->278 0.25448
266 ->279 0.31681
267 ->278 0.31680
267 ->279 -0.25448
268 ->277 -0.16754
269 ->281 -0.16235
270 ->282 0.14961
271 ->283 -0.14961
272 ->280 -0.16490

Excited state symmetry could not be determined.
Excited State 84: Singlet-?Sym 2.6722 eV 463.98 nm f=0.0005 <S**2>=0.000
266 ->278 0.37348
266 ->279 -0.32587
267 ->278 -0.32587
267 ->279 -0.37348

Excited state symmetry could not be determined.
Excited State 85: Singlet-?Sym 2.6730 eV 463.83 nm f=0.0000 <S**2>=0.000
266 ->278 0.45300
266 ->279 -0.19280
267 ->278 0.19281
267 ->279 0.45300

Excited State 86: Singlet-E 2.7309 eV 454.00 nm f=0.0387 <S**2>=0.000
245 ->274 -0.16546
248 ->274 0.65645
248 ->275 0.12372
258 ->276 -0.11814

Excited State 87: Singlet-E 2.7309 eV 454.00 nm f=0.0387 <S**2>=0.000
245 ->275 -0.16545
248 ->274 0.12372
248 ->275 -0.65645
259 ->276 -0.11814

Excited state symmetry could not be determined.
Excited State 88: Singlet-?Sym 2.7384 eV 452.77 nm f=0.0000 <S**2>=0.000
246 ->274 0.36227
246 ->275 0.34130
247 ->274 -0.34128
247 ->275 0.36228

Excited state symmetry could not be determined.
Excited State 89: Singlet-?Sym 2.7417 eV 452.22 nm f=0.0000 <S**2>=0.000
246 ->274 0.38206
246 ->275 -0.30134
247 ->274 -0.30136
247 ->275 -0.38204
260 ->276 -0.10450

Excited State 90: Singlet-B 2.7511 eV 450.68 nm f=0.0001 <S**2>=0.000
268 ->281 -0.13014
270 ->283 -0.15033
271 ->282 -0.15033
272 ->284 0.20239
273 ->280 0.56479
273 ->284 0.11330

Excited State 91: Singlet-E 2.7535 eV 450.28 nm f=0.0008 <S**2>=0.000
268 ->283 -0.14066

271 ->284 0.20364
272 ->282 -0.12706
273 ->283 0.57427

Excited State 92: Singlet-E 2.7535 eV 450.28 nm f=0.0008 <S**2>=0.000
268 ->282 0.14066
270 ->284 -0.20364
272 ->283 0.12706
273 ->282 0.57427

Excited State 93: Singlet-A 2.7547 eV 450.08 nm f=0.0000 <S**2>=0.000
268 ->280 -0.16920
269 ->284 0.22560
273 ->281 0.59149

Excited State 94: Singlet-B 2.7591 eV 449.36 nm f=0.0045 <S**2>=0.000
246 ->274 -0.28126
246 ->275 0.27807
247 ->274 -0.27806
247 ->275 -0.28128
272 ->280 -0.13953
273 ->280 -0.10027
273 ->284 0.32019

Excited state symmetry could not be determined.
Excited State 95: Singlet-?Sym 2.7604 eV 449.16 nm f=0.0000 <S**2>=0.000
246 ->274 0.27349
246 ->275 0.38459
247 ->274 0.38461
247 ->275 -0.27348
260 ->276 -0.18879

Excited State 96: Singlet-E 2.7639 eV 448.58 nm f=0.0579 <S**2>=0.000
245 ->274 0.48393
245 ->275 -0.36890
248 ->275 0.10429
249 ->274 -0.22466
258 ->276 -0.15923

Excited State 97: Singlet-E 2.7639 eV 448.58 nm f=0.0578 <S**2>=0.000
245 ->274 0.36891
245 ->275 0.48394
248 ->274 0.10429
249 ->275 -0.22463
259 ->276 -0.15920

Excited State 98: Singlet-B 2.7650 eV 448.40 nm f=0.0001 <S**2>=0.000
269 ->281 -0.18941
270 ->282 0.23642
271 ->283 -0.23642
272 ->280 0.56625

Excited State 99: Singlet-A 2.7652 eV 448.37 nm f=0.0000 <S**2>=0.000
269 ->280 0.50427
270 ->282 -0.10277
270 ->283 0.17261
271 ->282 -0.17261
271 ->283 -0.10276
272 ->281 -0.38767

Excited State 100: Singlet-E 2.7657 eV 448.29 nm f=0.0001 <S**2>=0.000
269 ->282 0.13893
269 ->283 -0.18754
270 ->281 -0.12542
271 ->280 0.57052
272 ->283 -0.30118

Table S5: Vertical Excitation energies of TAP^{Fc}Mg using B3LYP PCM-TDDFT

Excited State 1: Singlet-E 1.7210 eV 720.42 nm f=0.2321 <S**2>=0.000
241 ->251 0.15226
246 ->252 -0.11128
246 ->260 -0.10745
247 ->253 -0.13974
248 ->250 0.25829
248 ->251 -0.13392
248 ->254 -0.10739
249 ->251 0.50359
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3090.27227420
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-E 1.7210 eV 720.42 nm f=0.2321 <S**2>=0.000
241 ->250 0.15226
246 ->253 -0.13974
247 ->252 -0.11128
247 ->260 -0.10745

248 ->250 0.13392
248 ->251 0.25829
248 ->255 0.10739
249 ->250 0.50359

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 1.7573 eV 705.56 nm f=0.0016 <S**2>=0.000
242 ->253 -0.16536
243 ->250 0.35903
243 ->251 0.11404
243 ->254 -0.15572
244 ->250 0.11404
244 ->251 -0.35903
244 ->255 -0.15572
245 ->252 -0.15306
245 ->260 -0.14100
246 ->251 0.11586
246 ->259 -0.10175
247 ->250 0.11586
247 ->258 0.10175
248 ->257 -0.10347

Excited State 4: Singlet-E 1.7575 eV 705.46 nm f=0.0013 <S**2>=0.000
242 ->250 0.30337
242 ->251 -0.25221
242 ->254 -0.10343
242 ->255 -0.12612
244 ->252 0.15543
244 ->253 -0.14729
244 ->260 0.14250
245 ->250 -0.10943
245 ->251 0.37764
245 ->255 0.16421
247 ->257 -0.10330
248 ->258 0.10755

Excited State 5: Singlet-E 1.7575 eV 705.46 nm f=0.0013 <S**2>=0.000
242 ->250 0.25221
242 ->251 0.30337
242 ->254 -0.12612
242 ->255 0.10343
243 ->252 -0.15543
243 ->253 -0.14729
243 ->260 -0.14250
245 ->250 0.37764

245 ->251 0.10943
245 ->254 -0.16421
246 ->257 -0.10330
248 ->259 -0.10755

Excited state symmetry could not be determined.
Excited State 6: Singlet-?Sym 1.7579 eV 705.31 nm f=0.0000 <S**2>=0.000
242 ->252 0.15468
242 ->260 0.14218
243 ->250 -0.26802
243 ->251 -0.28529
243 ->254 0.13210
244 ->250 0.28529
244 ->251 -0.26802
244 ->255 -0.13210
245 ->253 0.17353
248 ->256 0.10752

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 1.7740 eV 698.90 nm f=0.0168 <S**2>=0.000
242 ->257 0.10445
243 ->250 -0.10566
244 ->251 0.10566
245 ->256 0.10778
246 ->250 0.14035
246 ->251 0.34870
246 ->255 0.13017
247 ->250 0.34870
247 ->251 -0.14035
247 ->254 -0.13017
248 ->253 -0.15686
249 ->252 -0.10710
249 ->260 -0.10680

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 1.7963 eV 690.24 nm f=0.0000 <S**2>=0.000
241 ->253 -0.12482
242 ->256 0.11507
243 ->259 0.11081
244 ->258 0.11081
245 ->257 0.11577
246 ->250 0.38435
246 ->254 -0.15906
247 ->251 0.38435
247 ->255 0.15906

248 ->252 -0.13340
248 ->260 -0.14579
249 ->253 -0.12685

Excited State 9: Singlet-E 1.9183 eV 646.33 nm f=0.0422 <S**2>=0.000
248 ->250 0.40541
248 ->251 0.32442
249 ->250 -0.35915
249 ->251 -0.22320

Excited State 10: Singlet-E 1.9183 eV 646.33 nm f=0.0422 <S**2>=0.000
248 ->250 -0.32442
248 ->251 0.40541
249 ->250 -0.22320
249 ->251 0.35915

Excited state symmetry could not be determined.
Excited State 11: Singlet-?Sym 2.0058 eV 618.12 nm f=0.0000 <S**2>=0.000
246 ->251 -0.49418
247 ->250 0.49418

Excited state symmetry could not be determined.
Excited State 12: Singlet-?Sym 2.0128 eV 615.97 nm f=0.0000 <S**2>=0.000
246 ->250 0.46326
246 ->251 -0.18334
247 ->250 -0.18334
247 ->251 -0.46326

Excited State 13: Singlet-E 2.0909 eV 592.97 nm f=0.0150 <S**2>=0.000
242 ->250 0.41440
242 ->251 0.25595
245 ->250 -0.38811
245 ->251 -0.30777

Excited State 14: Singlet-E 2.0909 eV 592.97 nm f=0.0150 <S**2>=0.000
242 ->250 -0.25595
242 ->251 0.41440
245 ->250 -0.30777
245 ->251 0.38811

Excited state symmetry could not be determined.
Excited State 15: Singlet-?Sym 2.0929 eV 592.41 nm f=0.0014 <S**2>=0.000
243 ->250 -0.17758
243 ->251 0.45831
244 ->250 0.45831

244 ->251 0.17758

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 2.0944 eV 591.97 nm f=0.0000 <S**2>=0.000
243 ->250 0.37402
243 ->251 -0.32934
244 ->250 0.32934
244 ->251 0.37402

Excited State 17: Singlet-E 2.1438 eV 578.33 nm f=0.1456 <S**2>=0.000
241 ->250 -0.19619
241 ->254 0.10072
242 ->259 -0.19235
243 ->256 -0.18469
243 ->257 -0.13197
244 ->257 0.15136
245 ->258 0.16794
245 ->259 -0.10787
246 ->253 0.15810
247 ->260 0.13878
248 ->250 0.11140
248 ->251 0.32426
248 ->255 -0.13512
249 ->250 0.18259
249 ->254 0.11846

Excited State 18: Singlet-E 2.1438 eV 578.33 nm f=0.1456 <S**2>=0.000
241 ->251 -0.19619
241 ->255 -0.10072
242 ->258 0.19235
243 ->257 -0.15136
244 ->256 0.18469
244 ->257 -0.13197
245 ->258 -0.10787
245 ->259 -0.16794
246 ->260 0.13878
247 ->253 0.15810
248 ->250 0.32426
248 ->251 -0.11140
248 ->254 0.13512
249 ->251 0.18259
249 ->255 -0.11846

Excited state symmetry could not be determined.
Excited State 19: Singlet-?Sym 2.1794 eV 568.89 nm f=0.0081 <S**2>=0.000

241 ->260 0.10143
242 ->257 -0.22892
243 ->258 0.13769
243 ->259 -0.18099
244 ->258 0.18099
244 ->259 0.13769
245 ->256 -0.22652
246 ->251 0.25147
246 ->255 -0.13413
247 ->250 0.25147
247 ->254 0.13413
248 ->253 0.16270
249 ->260 0.12107

Excited state symmetry could not be determined.
Excited State 20: Singlet-?Sym 2.1916 eV 565.72 nm f=0.0000 <S**2>=0.000
242 ->256 -0.23074
243 ->259 -0.22384
244 ->258 -0.22384
245 ->257 -0.22867
246 ->250 0.28751
246 ->254 0.14935
247 ->251 0.28751
247 ->255 -0.14935
248 ->260 0.14661
249 ->253 0.12950

Excited State 21: Singlet-E 2.1989 eV 563.85 nm f=0.0002 <S**2>=0.000
241 ->259 0.14540
242 ->250 0.24092
242 ->251 0.14913
242 ->254 0.14276
243 ->253 0.15221
243 ->260 0.14465
245 ->250 0.19078
245 ->251 0.17114
245 ->254 0.14371
246 ->256 0.20301
246 ->257 0.18237
247 ->256 0.11190
247 ->257 0.14834
248 ->258 -0.11442
248 ->259 0.20396
249 ->259 0.17288

Excited State 22: Singlet-E 2.1989 eV 563.85 nm f=0.0002 <S**2>=0.000

241 ->258	-0.14540
242 ->250	-0.14913
242 ->251	0.24092
242 ->255	-0.14276
244 ->253	-0.15221
244 ->260	0.14465
245 ->250	0.17114
245 ->251	-0.19078
245 ->255	0.14371
246 ->256	-0.11190
246 ->257	0.14834
247 ->256	0.20301
247 ->257	-0.18237
248 ->258	0.20396
248 ->259	0.11442
249 ->258	-0.17288

Excited State 23: Singlet-A 2.2001 eV 563.54 nm f=0.0000 <S**2>=0.000

241 ->257	0.15764
242 ->260	0.15271
243 ->250	0.16869
243 ->251	0.21191
243 ->254	0.12806
244 ->250	-0.21191
244 ->251	0.16869
244 ->255	-0.12806
245 ->253	0.15467
246 ->258	-0.19837
246 ->259	0.12656
247 ->258	0.12656
247 ->259	0.19837
248 ->256	0.23607
249 ->257	0.18841

Excited state symmetry could not be determined.

Excited State 24: Singlet-?Sym 2.2006 eV 563.42 nm f=0.0000 <S**2>=0.000

241 ->256	0.15739
242 ->253	0.15644
243 ->250	0.25072
243 ->251	0.11148
243 ->254	0.15196
244 ->250	0.11148
244 ->251	-0.25072
244 ->255	0.15196

245 ->260 0.15042
246 ->259 0.22921
247 ->258 -0.22921
248 ->257 0.23569
249 ->256 0.18814

Excited State 25: Singlet-E 2.2911 eV 541.16 nm f=0.1330 <S**2>=0.000
241 ->250 0.55050
241 ->251 0.28937
242 ->259 -0.11542
243 ->256 -0.12034
243 ->257 -0.11052
245 ->259 -0.10294

Excited State 26: Singlet-E 2.2911 eV 541.16 nm f=0.1330 <S**2>=0.000
241 ->250 -0.28937
241 ->251 0.55050
242 ->258 0.11542
244 ->256 0.12034
244 ->257 -0.11052
245 ->258 -0.10294

Excited State 27: Singlet-B 2.4613 eV 503.73 nm f=0.0004 <S**2>=0.000
233 ->250 0.16627
233 ->254 -0.15735
233 ->255 -0.13705
234 ->251 -0.16627
234 ->254 0.13705
234 ->255 -0.15735
235 ->253 0.21591
236 ->252 0.12521
236 ->260 0.17942
242 ->257 -0.14646
243 ->259 -0.11427
244 ->258 0.11427
245 ->256 -0.14644
246 ->255 0.12693
247 ->254 -0.12693
248 ->253 -0.15911
249 ->252 -0.11265
249 ->260 -0.12954

Excited State 28: Singlet-E 2.4648 eV 503.02 nm f=0.0050 <S**2>=0.000
233 ->253 0.20504
234 ->252 -0.12637

234 ->260 -0.17727
235 ->250 0.18467
235 ->254 -0.18655
236 ->251 0.17003
236 ->255 0.18022
240 ->250 0.12473
241 ->251 0.11624
242 ->258 -0.13003
243 ->257 0.11623
244 ->256 -0.12141
245 ->259 0.12700
246 ->260 0.14062
247 ->253 0.15683
248 ->254 0.14162
249 ->255 -0.13463

Excited State 29: Singlet-E 2.4648 eV 503.02 nm f=0.0050 <S**2>=0.000
233 ->252 -0.12637
233 ->260 -0.17727
234 ->253 0.20504
235 ->251 -0.18467
235 ->255 -0.18655
236 ->250 -0.17003
236 ->254 0.18022
240 ->251 -0.12473
241 ->250 -0.11624
242 ->259 -0.13003
243 ->256 -0.12141
244 ->257 0.11623
245 ->258 0.12700
246 ->253 -0.15683
247 ->260 -0.14062
248 ->255 0.14162
249 ->254 -0.13463

Excited state symmetry could not be determined.
Excited State 30: Singlet-?Sym 2.4652 eV 502.94 nm f=0.0000 <S**2>=0.000
233 ->251 0.19242
233 ->255 0.20988
234 ->250 -0.19242
234 ->254 0.20988
235 ->252 0.13824
235 ->260 0.19401
236 ->253 0.20309
242 ->256 -0.13889

243 ->259 -0.13630
244 ->258 -0.13630
245 ->257 -0.13887
246 ->250 -0.10863
246 ->254 -0.15681
247 ->251 -0.10863
247 ->255 0.15681
248 ->252 -0.10265
248 ->260 -0.14974
249 ->253 -0.15068

Excited State 31: Singlet-E 2.5042 eV 495.10 nm f=0.0486 <S**2>=0.000
240 ->250 0.58233
240 ->251 0.33751

Excited State 32: Singlet-E 2.5042 eV 495.10 nm f=0.0486 <S**2>=0.000
240 ->250 -0.33751
240 ->251 0.58233

Excited state symmetry could not be determined.
Excited State 33: Singlet-?Sym 2.5208 eV 491.85 nm f=0.0157 <S**2>=0.000
238 ->250 0.34128
238 ->251 -0.34731
239 ->250 0.34731
239 ->251 0.34128

Excited state symmetry could not be determined.
Excited State 34: Singlet-?Sym 2.5493 eV 486.35 nm f=0.0000 <S**2>=0.000
238 ->251 0.48874
239 ->250 0.48874

Excited State 35: Singlet-B 2.5725 eV 481.95 nm f=0.0000 <S**2>=0.000
233 ->258 0.21263
234 ->259 0.21263
235 ->257 0.21570
236 ->256 0.19893
241 ->256 0.12734
242 ->253 -0.19507
243 ->250 -0.10775
243 ->254 -0.19022
244 ->251 0.10775
244 ->255 -0.19022
245 ->252 -0.12004
245 ->260 -0.17821
246 ->259 0.15238

247 ->258 -0.15238
248 ->257 0.15333
249 ->256 0.11041

Excited State 36: Singlet-A 2.5730 eV 481.87 nm f=0.0000 <S**2>=0.000
233 ->258 -0.13466
233 ->259 -0.16497
234 ->258 -0.16497
234 ->259 0.13466
235 ->256 0.21561
236 ->257 0.19900
241 ->257 0.12708
242 ->252 -0.12024
242 ->260 -0.17864
243 ->254 -0.15473
243 ->255 0.11021
244 ->254 0.11021
244 ->255 0.15473
245 ->253 -0.19483
246 ->258 -0.12847
247 ->259 0.12847
248 ->256 0.15355
249 ->257 0.11026

Excited State 37: Singlet-E 2.5730 eV 481.86 nm f=0.0002 <S**2>=0.000
233 ->256 -0.13837
234 ->256 0.16529
234 ->257 0.20929
235 ->259 0.21028
236 ->258 -0.11835
236 ->259 0.15818
241 ->259 0.10018
242 ->254 -0.15811
242 ->255 0.10815
243 ->252 -0.12050
243 ->253 -0.17432
243 ->260 -0.17859
245 ->250 -0.10632
245 ->254 -0.18861
246 ->256 0.10656
246 ->257 0.14590
247 ->256 0.11401
248 ->259 0.15000

Excited State 38: Singlet-E 2.5730 eV 481.86 nm f=0.0002 <S**2>=0.000

233 ->256 -0.16529
233 ->257 0.20929
234 ->256 -0.13837
235 ->258 0.21028
236 ->258 -0.15818
236 ->259 -0.11835
241 ->258 -0.10018
242 ->254 0.10815
242 ->255 0.15811
244 ->252 -0.12050
244 ->253 0.17432
244 ->260 -0.17859
245 ->251 0.10632
245 ->255 -0.18861
246 ->256 -0.11401
247 ->256 0.10656
247 ->257 -0.14590
248 ->258 0.15000

Excited state symmetry could not be determined.
Excited State 39: Singlet-?Sym 2.6284 eV 471.70 nm f=0.0001 <S**2>=0.000
238 ->250 0.35494
238 ->251 0.34712
239 ->250 -0.34712
239 ->251 0.35494

Excited state symmetry could not be determined.
Excited State 40: Singlet-?Sym 2.6394 eV 469.75 nm f=0.0000 <S**2>=0.000
238 ->250 -0.49569
239 ->251 0.49569

Excited State 41: Singlet-E 2.8736 eV 431.46 nm f=0.0804 <S**2>=0.000
228 ->250 0.15066
232 ->250 -0.26558
236 ->250 0.13305
237 ->250 0.26103
237 ->251 0.54241
240 ->250 0.10263

Excited State 42: Singlet-E 2.8736 eV 431.46 nm f=0.0804 <S**2>=0.000
228 ->251 -0.15066
232 ->251 0.26558
236 ->251 -0.13305
237 ->250 0.54241
237 ->251 -0.26103

240 ->251 0.10263

Excited State 43: Singlet-E 2.9429 eV 421.29 nm f=0.0008 <S**2>=0.000
227 ->250 0.61915
228 ->250 0.27608
232 ->250 0.16280

Excited State 44: Singlet-E 2.9429 eV 421.29 nm f=0.0008 <S**2>=0.000
227 ->251 0.61915
228 ->251 0.27608
232 ->251 0.16280

Excited state symmetry could not be determined.
Excited State 45: Singlet-?Sym 3.0354 eV 408.46 nm f=0.0042 <S**2>=0.000
233 ->250 0.34184
233 ->251 -0.20866
234 ->250 -0.20866
234 ->251 -0.34184
242 ->257 0.13589
243 ->259 0.10605
244 ->258 -0.10605
245 ->256 0.13572
248 ->253 0.11108
249 ->252 0.20828

Excited state symmetry could not be determined.
Excited State 46: Singlet-?Sym 3.0430 eV 407.44 nm f=0.0000 <S**2>=0.000
233 ->251 -0.40638
234 ->250 0.40638
242 ->256 -0.13763
243 ->259 -0.13478
244 ->258 -0.13478
245 ->257 -0.13742
246 ->254 -0.11797
247 ->255 0.11797
248 ->252 -0.14534
248 ->260 -0.10688
249 ->253 -0.10638

Excited State 47: Singlet-E 3.0437 eV 407.35 nm f=0.0074 <S**2>=0.000
232 ->250 0.14836
235 ->250 0.18624
235 ->251 0.36858
236 ->250 0.36443
242 ->259 -0.13430

243 ->256 -0.13072
245 ->258 0.11196
246 ->253 -0.12227
247 ->252 -0.13261
249 ->254 -0.10508

Excited State 48: Singlet-E 3.0437 eV 407.35 nm f=0.0074 <S**2>=0.000
232 ->251 0.14836
235 ->250 0.36858
235 ->251 -0.18624
236 ->251 0.36443
242 ->258 0.13430
244 ->256 0.13072
245 ->259 -0.11196
246 ->252 -0.13261
247 ->253 -0.12227
249 ->255 0.10508

Excited state symmetry could not be determined.
Excited State 49: Singlet-?Sym 3.1745 eV 390.57 nm f=0.0000 <S**2>=0.000
233 ->250 0.24493
233 ->251 0.42346
234 ->250 0.42346
234 ->251 -0.24493

Excited state symmetry could not be determined.
Excited State 50: Singlet-?Sym 3.1751 eV 390.49 nm f=0.0000 <S**2>=0.000
233 ->250 0.48768
234 ->251 0.48768

Excited State 51: Singlet-E 3.1763 eV 390.34 nm f=0.0050 <S**2>=0.000
232 ->250 -0.10325
235 ->250 0.45050
235 ->251 0.18204
236 ->250 -0.33659
236 ->251 -0.34204

Excited State 52: Singlet-E 3.1763 eV 390.34 nm f=0.0050 <S**2>=0.000
232 ->251 0.10325
235 ->250 -0.18204
235 ->251 0.45050
236 ->250 -0.34204
236 ->251 0.33659

Excited state symmetry could not be determined.

Excited State 53: Singlet-?Sym 3.1855 eV 389.22 nm f=0.0000 <S**2>=0.000
230 ->250 -0.22890
230 ->251 -0.42727
231 ->250 0.42727
231 ->251 -0.22890

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 3.1855 eV 389.22 nm f=0.0001 <S**2>=0.000
230 ->250 -0.48410
231 ->251 0.48410

Excited State 55: Singlet-E 3.1920 eV 388.42 nm f=0.0076 <S**2>=0.000
227 ->250 0.13004
227 ->251 -0.17120
228 ->250 -0.20725
228 ->251 0.17612
229 ->250 -0.19777
229 ->251 0.44633
232 ->250 -0.12991
232 ->251 0.31108

Excited State 56: Singlet-E 3.1920 eV 388.42 nm f=0.0076 <S**2>=0.000
227 ->250 0.17120
227 ->251 0.13004
228 ->250 -0.17612
228 ->251 -0.20725
229 ->250 0.44633
229 ->251 0.19777
232 ->250 -0.31108
232 ->251 -0.12991

Excited State 57: Singlet-B 3.2556 eV 380.83 nm f=0.0119 <S**2>=0.000
230 ->251 0.38807
231 ->250 0.38807
249 ->252 0.38897

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 3.2609 eV 380.21 nm f=0.0000 <S**2>=0.000
230 ->250 0.43446
230 ->251 -0.23108
231 ->250 0.23108
231 ->251 0.43446

Excited State 59: Singlet-E 3.2671 eV 379.50 nm f=0.0545 <S**2>=0.000
227 ->250 -0.10406

227 ->251 -0.16092
228 ->251 0.24641
229 ->250 0.50194
232 ->250 0.23181
232 ->251 0.24300
237 ->251 0.10678

Excited State 60: Singlet-E 3.2671 eV 379.50 nm f=0.0545 <S**2>=0.000
227 ->250 -0.16092
227 ->251 0.10406
228 ->250 0.24641
229 ->251 0.50194
232 ->250 0.24300
232 ->251 -0.23181
237 ->250 0.10678

Excited State 61: Singlet-B 3.2697 eV 379.19 nm f=0.0467 <S**2>=0.000
230 ->251 -0.29480
231 ->250 -0.29480
249 ->252 0.51372

Excited state symmetry could not be determined.
Excited State 62: Singlet-?Sym 3.3534 eV 369.72 nm f=0.0010 <S**2>=0.000
217 ->251 0.24813
218 ->250 0.24813
221 ->250 0.11269
221 ->251 0.37332
222 ->250 0.37332
222 ->251 -0.11269
227 ->252 -0.13983

Excited state symmetry could not be determined.
Excited State 63: Singlet-?Sym 3.3665 eV 368.29 nm f=0.0000 <S**2>=0.000
217 ->250 0.23657
218 ->251 0.23657
221 ->250 0.35271
221 ->251 0.20280
222 ->250 -0.20280
222 ->251 0.35271

Excited State 64: Singlet-B 3.4137 eV 363.20 nm f=0.0000 <S**2>=0.000
217 ->250 0.15372
218 ->251 -0.15372
221 ->250 0.27330
222 ->251 -0.27330

233 ->258 0.16414
234 ->259 0.16414
235 ->257 0.16603
236 ->256 0.15455
245 ->252 0.31307
249 ->256 -0.10415

Excited State 65: Singlet-E 3.4169 eV 362.85 nm f=0.0034 <S**2>=0.000
233 ->256 -0.14035
233 ->257 0.22370
234 ->256 -0.17443
235 ->258 0.22256
236 ->258 -0.13908
236 ->259 -0.15282
244 ->252 0.41226
246 ->256 0.11286
247 ->257 0.13056
248 ->258 -0.13427
249 ->259 0.10470

Excited State 66: Singlet-E 3.4169 eV 362.85 nm f=0.0034 <S**2>=0.000
233 ->256 -0.17443
234 ->256 0.14035
234 ->257 0.22370
235 ->259 0.22256
236 ->258 -0.15282
236 ->259 0.13908
243 ->252 0.41226
246 ->257 -0.13056
247 ->256 -0.11286
248 ->259 -0.13427
249 ->258 0.10470

Excited State 67: Singlet-A 3.4176 eV 362.78 nm f=0.0000 <S**2>=0.000
217 ->251 -0.14785
218 ->250 0.14785
221 ->251 -0.19403
222 ->250 0.19403
233 ->258 -0.11856
233 ->259 -0.14143
234 ->258 -0.14143
234 ->259 0.11856
235 ->256 0.18721
236 ->257 0.17463
242 ->252 0.35190

248 ->256 -0.11329
249 ->257 -0.11757

Excited state symmetry could not be determined.
Excited State 68: Singlet-?Sym 3.4205 eV 362.47 nm f=0.0000 <S**2>=0.000
217 ->250 0.10338
217 ->251 -0.19962
218 ->250 0.19962
218 ->251 0.10338
221 ->250 0.17642
221 ->251 -0.27538
222 ->250 0.27538
222 ->251 0.17642
235 ->256 -0.12179
236 ->257 -0.11313
242 ->252 -0.22948

Excited State 69: Singlet-B 3.4208 eV 362.44 nm f=0.0001 <S**2>=0.000
217 ->250 -0.20718
218 ->251 0.20718
221 ->250 -0.28288
222 ->251 0.28288
233 ->258 0.14617
234 ->259 0.14617
235 ->257 0.14867
236 ->256 0.13845
245 ->252 0.29361

Excited State 70: Singlet-E 3.4303 eV 361.44 nm f=0.2475 <S**2>=0.000
228 ->250 0.14727
228 ->251 -0.18692
232 ->251 0.16474
234 ->253 0.11029
234 ->260 0.10785
235 ->250 0.10188
235 ->254 0.11918
236 ->250 0.11581
236 ->254 0.10407
237 ->250 -0.11459
246 ->252 0.41428
247 ->252 0.27872

Excited State 71: Singlet-E 3.4303 eV 361.44 nm f=0.2475 <S**2>=0.000
228 ->250 -0.18692
228 ->251 -0.14727

232 ->250 0.16474
233 ->253 0.11029
233 ->260 -0.10785
235 ->251 0.10188
235 ->255 -0.11918
236 ->251 -0.11581
236 ->255 0.10407
237 ->251 0.11459
246 ->252 -0.27872
247 ->252 0.41428

Excited State 72: Singlet-A 3.4406 eV 360.36 nm f=0.0000 <S**2>=0.000
233 ->251 -0.14817
233 ->255 0.14979
234 ->250 0.14817
234 ->254 0.14979
235 ->260 0.14392
236 ->253 0.14187
248 ->252 0.54318

Excited State 73: Singlet-E 3.4923 eV 355.02 nm f=0.4801 <S**2>=0.000
223 ->251 -0.19287
226 ->250 -0.13026
226 ->251 0.17068
228 ->251 0.32577
232 ->251 -0.17920
233 ->260 -0.11353
234 ->253 0.11933
235 ->255 -0.11516
236 ->250 0.13570
236 ->254 0.10669
237 ->250 0.16543
237 ->251 -0.16056
238 ->252 -0.10059
246 ->252 0.10240

Excited State 74: Singlet-E 3.4923 eV 355.02 nm f=0.4801 <S**2>=0.000
223 ->250 -0.19287
226 ->250 -0.17068
226 ->251 -0.13026
228 ->250 0.32577
232 ->250 -0.17920
233 ->253 0.11933
234 ->260 -0.11353
235 ->254 -0.11516

236 ->251 -0.13570
236 ->255 0.10669
237 ->250 -0.16056
237 ->251 -0.16543
239 ->252 0.10059
247 ->252 0.10240

Excited State 75: Singlet-B 3.5022 eV 354.02 nm f=0.0003 <S**2>=0.000
224 ->250 0.16078
224 ->251 -0.15080
225 ->250 0.15080
225 ->251 0.16078
233 ->250 -0.14112
233 ->254 -0.15195
233 ->255 -0.13130
234 ->251 0.14112
234 ->254 0.13130
234 ->255 -0.15195
235 ->253 0.20466
236 ->252 0.10029
236 ->260 0.17729
241 ->252 0.24628
242 ->257 0.10685
245 ->256 0.10803

Excited state symmetry could not be determined.
Excited State 76: Singlet-?Sym 3.5421 eV 350.03 nm f=0.0000 <S**2>=0.000
224 ->251 0.38243
225 ->250 0.38243
248 ->252 -0.27761

Excited State 77: Singlet-E 3.5682 eV 347.47 nm f=0.1771 <S**2>=0.000
223 ->251 0.25872
226 ->250 0.35439
226 ->251 -0.27163
228 ->250 0.10159
228 ->251 0.11923
246 ->252 -0.27766

Excited State 78: Singlet-E 3.5682 eV 347.47 nm f=0.1771 <S**2>=0.000
223 ->250 0.25872
226 ->250 0.27163
226 ->251 0.35439
228 ->250 0.11923
228 ->251 -0.10159

247 ->252 -0.27766

Excited state symmetry could not be determined.
Excited State 79: Singlet-?Sym 3.5743 eV 346.88 nm f=0.0149 <S**2>=0.000
224 ->250 0.32147
224 ->251 -0.26577
225 ->250 0.26577
225 ->251 0.32147
241 ->252 -0.16330
245 ->252 -0.13585

Excited State 80: Singlet-E 3.5873 eV 345.62 nm f=0.0027 <S**2>=0.000
219 ->251 0.10005
233 ->256 0.10178
233 ->257 -0.11627
235 ->258 -0.11773
242 ->255 0.13235
244 ->252 0.50575
244 ->253 0.14396
244 ->260 -0.16323
245 ->255 -0.14508

Excited State 81: Singlet-E 3.5873 eV 345.62 nm f=0.0027 <S**2>=0.000
219 ->250 -0.10005
234 ->256 -0.10178
234 ->257 -0.11627
235 ->259 -0.11773
242 ->254 -0.13235
243 ->252 0.50575
243 ->253 -0.14396
243 ->260 -0.16323
245 ->254 -0.14508

Excited State 82: Singlet-B 3.5876 eV 345.59 nm f=0.0015 <S**2>=0.000
233 ->258 -0.12349
234 ->259 -0.12349
235 ->257 -0.12417
236 ->256 -0.11590
242 ->253 -0.15154
243 ->254 -0.14442
244 ->255 -0.14442
245 ->252 0.49174
245 ->260 -0.16355

Excited State 83: Singlet-A 3.5883 eV 345.52 nm f=0.0000 <S**2>=0.000

235 ->256 -0.12410
236 ->257 -0.11573
242 ->252 0.50970
242 ->260 -0.16429
243 ->254 -0.12278
244 ->255 0.12278
245 ->253 -0.15675

Excited state symmetry could not be determined.
Excited State 84: Singlet-?Sym 3.6011 eV 344.30 nm f=0.0000 <S**2>=0.000
224 ->251 0.26798
225 ->250 0.26798
233 ->251 0.12446
233 ->255 -0.16248
234 ->250 -0.12446
234 ->254 -0.16248
235 ->260 -0.15237
236 ->253 -0.15406
242 ->256 -0.10419
243 ->259 -0.10238
244 ->258 -0.10238
245 ->257 -0.10535
246 ->254 -0.12212
247 ->255 0.12212
248 ->252 0.23690
248 ->260 -0.12278
249 ->253 -0.11323

Excited State 85: Singlet-E 3.6163 eV 342.85 nm f=0.0696 <S**2>=0.000
226 ->250 0.18276
226 ->251 0.34873
228 ->250 0.12180
232 ->250 -0.13947
233 ->260 0.12675
234 ->253 -0.10373
235 ->251 -0.10104
235 ->255 0.13744
246 ->252 -0.11403
247 ->252 0.25819
247 ->260 -0.10656
248 ->255 0.11382

Excited State 86: Singlet-E 3.6163 eV 342.85 nm f=0.0696 <S**2>=0.000
226 ->250 0.34873
226 ->251 -0.18276

228 ->251 0.12180
232 ->251 -0.13947
233 ->253 0.10373
234 ->260 -0.12675
235 ->250 -0.10104
235 ->254 -0.13744
246 ->252 0.25819
246 ->260 -0.10656
247 ->252 0.11403
248 ->254 -0.11382

Excited state symmetry could not be determined.
Excited State 87: Singlet-?Sym 3.6430 eV 340.33 nm f=0.0000 <S**2>=0.000
221 ->250 0.10136
222 ->251 -0.10136
224 ->250 -0.31546
224 ->251 -0.36873
225 ->250 0.36873
225 ->251 -0.31546

Excited state symmetry could not be determined.
Excited State 88: Singlet-?Sym 3.6474 eV 339.93 nm f=0.0000 <S**2>=0.000
224 ->250 -0.48310
225 ->251 0.48310

Excited State 89: Singlet-E 3.6583 eV 338.91 nm f=0.0784 <S**2>=0.000
223 ->250 -0.28395
223 ->251 0.53602
226 ->250 -0.11129
226 ->251 0.26459

Excited State 90: Singlet-E 3.6583 eV 338.91 nm f=0.0784 <S**2>=0.000
223 ->250 0.53602
223 ->251 0.28395
226 ->250 -0.26459
226 ->251 -0.11129

Excited State 91: Singlet-B 3.7193 eV 333.35 nm f=0.0057 <S**2>=0.000
241 ->252 0.60662
248 ->253 -0.11236
249 ->260 -0.10868

Excited State 92: Singlet-E 3.7286 eV 332.53 nm f=0.0170 <S**2>=0.000
219 ->250 0.22681
219 ->251 -0.36764

220 ->250 -0.25824
220 ->251 0.43905

Excited State 93: Singlet-E 3.7286 eV 332.53 nm f=0.0170 <S**2>=0.000
219 ->250 0.36764
219 ->251 0.22681
220 ->250 0.43905
220 ->251 0.25824

Excited state symmetry could not be determined.
Excited State 94: Singlet-?Sym 3.7451 eV 331.06 nm f=0.0000 <S**2>=0.000
217 ->250 0.40651
218 ->251 0.40651
221 ->250 -0.23401
222 ->251 -0.23401

Excited state symmetry could not be determined.
Excited State 95: Singlet-?Sym 3.7457 eV 331.00 nm f=0.0000 <S**2>=0.000
217 ->250 0.21967
217 ->251 0.34000
218 ->250 0.34000
218 ->251 -0.21967
221 ->250 -0.17063
221 ->251 -0.17660
222 ->250 -0.17660
222 ->251 0.17063

Excited State 96: Singlet-E 3.8187 eV 324.68 nm f=0.0020 <S**2>=0.000
219 ->251 0.52282
220 ->250 -0.43163
220 ->251 0.14857

Excited State 97: Singlet-E 3.8187 eV 324.68 nm f=0.0020 <S**2>=0.000
219 ->250 0.52282
220 ->250 -0.14857
220 ->251 -0.43163

Excited state symmetry could not be determined.
Excited State 98: Singlet-?Sym 3.8375 eV 323.09 nm f=0.0000 <S**2>=0.000
217 ->251 -0.41810
218 ->250 0.41810
221 ->251 0.25266
222 ->250 -0.25266

Excited state symmetry could not be determined.

Excited State 99: Singlet-?Sym 3.8379 eV 323.05 nm f=0.0000 <S**2>=0.000
217 ->250 -0.35727
217 ->251 0.21379
218 ->250 0.21379
218 ->251 0.35727
221 ->250 0.18618
221 ->251 -0.19927
222 ->250 -0.19927
222 ->251 -0.18618

Excited State 100: Singlet-A 4.0079 eV 309.35 nm f=0.0000 <S**2>=0.000
240 ->252 0.68036

Table S6: Vertical Excitation energies of $TAP^{FcCN}Mg$ using B3LYP PCM-TDDFT

Excited State 1: Singlet-E 1.3898 eV 892.13 nm f=0.0035 <S**2>=0.000
266 ->274 0.33805
266 ->275 -0.29403
267 ->276 -0.14100
269 ->274 0.12767
269 ->275 0.43973
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3459.18228400
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-E 1.3898 eV 892.13 nm f=0.0035 <S**2>=0.000
266 ->274 0.29403
266 ->275 0.33805
268 ->276 0.14100
269 ->274 0.43973
269 ->275 -0.12767

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 1.3907 eV 891.50 nm f=0.0000 <S**2>=0.000
266 ->276 0.16758
267 ->274 -0.13420
267 ->275 0.43236
268 ->274 0.43221
268 ->275 0.13416
269 ->277 -0.10022

Excited state symmetry could not be determined.
Excited State 4: Singlet-?Sym 1.3909 eV 891.42 nm f=0.0001 <S**2>=0.000
266 ->277 -0.10013
267 ->274 0.11971

267 ->275 -0.43718
268 ->274 0.43734
268 ->275 0.11976
269 ->276 0.16799

Excited State 5: Singlet-E 1.4140 eV 876.84 nm f=0.2528 <S**2>=0.000
265 ->275 0.12250
270 ->276 0.10797
272 ->274 0.23867
272 ->275 -0.17053
273 ->274 0.20032
273 ->275 0.53688

Excited State 6: Singlet-E 1.4140 eV 876.84 nm f=0.2528 <S**2>=0.000
265 ->274 0.12250
271 ->276 0.10797
272 ->274 0.17053
272 ->275 0.23867
273 ->274 0.53688
273 ->275 -0.20032

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 1.4740 eV 841.13 nm f=0.0301 <S**2>=0.000
270 ->274 0.30861
270 ->275 0.33406
271 ->274 0.33406
271 ->275 -0.30861
273 ->276 0.11122

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 1.5016 eV 825.66 nm f=0.0000 <S**2>=0.000
270 ->274 0.43538
270 ->275 -0.13312
271 ->274 0.13312
271 ->275 0.43538
272 ->276 0.12861

Excited State 9: Singlet-E 1.5790 eV 785.22 nm f=0.0136 <S**2>=0.000
272 ->274 -0.26614
272 ->275 0.54035
273 ->275 0.34539

Excited State 10: Singlet-E 1.5790 eV 785.22 nm f=0.0136 <S**2>=0.000
272 ->274 0.54035
272 ->275 0.26614

273 ->274 -0.34539

Excited state symmetry could not be determined.
Excited State 11: Singlet-?Sym 1.6448 eV 753.81 nm f=0.0000 <S**2>=0.000
270 ->274 -0.13629
270 ->275 -0.47779
271 ->274 0.47779
271 ->275 -0.13629

Excited state symmetry could not be determined.
Excited State 12: Singlet-?Sym 1.6513 eV 750.83 nm f=0.0001 <S**2>=0.000
270 ->274 0.36515
270 ->275 -0.33970
271 ->274 -0.33970
271 ->275 -0.36515

Excited State 13: Singlet-E 1.7354 eV 714.45 nm f=0.0057 <S**2>=0.000
266 ->274 0.17463
266 ->275 0.46803
269 ->274 -0.40005
269 ->275 0.29460

Excited State 14: Singlet-E 1.7354 eV 714.45 nm f=0.0057 <S**2>=0.000
266 ->274 0.46803
266 ->275 -0.17463
269 ->274 -0.29460
269 ->275 -0.40005

Excited state symmetry could not be determined.
Excited State 15: Singlet-?Sym 1.7364 eV 714.04 nm f=0.0009 <S**2>=0.000
267 ->274 0.47715
267 ->275 0.13600
268 ->274 -0.13600
268 ->275 0.47714

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 1.7376 eV 713.55 nm f=0.0000 <S**2>=0.000
267 ->274 -0.47583
267 ->275 -0.15064
268 ->274 -0.15064
268 ->275 0.47583

Excited State 17: Singlet-E 1.9919 eV 622.45 nm f=0.3559 <S**2>=0.000
265 ->274 -0.36584
265 ->275 0.49591

272 ->275 0.14296
273 ->274 0.10151
273 ->275 -0.11648

Excited State 18: Singlet-E 1.9919 eV 622.45 nm f=0.3559 <S**2>=0.000
265 ->274 0.49591
265 ->275 0.36584
272 ->274 -0.14296
273 ->274 -0.11648
273 ->275 -0.10151

Excited State 19: Singlet-B 2.1115 eV 587.18 nm f=0.0032 <S**2>=0.000
266 ->281 0.21299
267 ->282 -0.21162
268 ->283 0.21166
269 ->280 0.13432
269 ->284 -0.16493
270 ->274 -0.12245
270 ->275 -0.13109
270 ->278 0.14243
270 ->287 -0.12883
271 ->274 -0.13109
271 ->275 0.12242
271 ->279 -0.14243
271 ->286 -0.12881
272 ->277 -0.15685
272 ->285 -0.14457
273 ->276 0.21962
273 ->280 -0.13037
273 ->284 -0.11111

Excited State 20: Singlet-A 2.1293 eV 582.27 nm f=0.0000 <S**2>=0.000
266 ->280 0.14805
266 ->284 -0.17018
267 ->282 0.22300
268 ->283 0.22297
269 ->281 0.22490
270 ->274 -0.18154
270 ->279 -0.15418
270 ->287 -0.11136
271 ->275 -0.18156
271 ->278 0.15419
271 ->286 0.11139
272 ->276 0.17774
272 ->280 -0.14351

272 ->284 -0.12812
273 ->277 -0.15010
273 ->285 -0.12925

Excited State 21: Singlet-E 2.1407 eV 579.18 nm f=0.0027 <S**2>=0.000
265 ->275 0.25128
266 ->282 0.21532
267 ->280 0.12395
267 ->281 -0.20907
267 ->284 -0.17698
269 ->282 -0.20397
271 ->276 0.12840
271 ->277 0.13458
271 ->280 -0.13019
271 ->285 0.12724
272 ->275 -0.13155
272 ->278 0.11164
272 ->286 0.13236
273 ->278 -0.12164
273 ->286 -0.11837

Excited State 22: Singlet-E 2.1407 eV 579.18 nm f=0.0027 <S**2>=0.000
265 ->274 0.25128
266 ->283 -0.21532
268 ->280 -0.12395
268 ->281 -0.20907
268 ->284 0.17698
269 ->283 -0.20397
270 ->276 -0.12840
270 ->277 0.13458
270 ->280 0.13019
270 ->285 0.12724
272 ->274 0.13155
272 ->279 0.11164
272 ->287 0.13236
273 ->279 0.12164
273 ->287 0.11837

Excited State 23: Singlet-B 2.1522 eV 576.09 nm f=0.0000 <S**2>=0.000
266 ->277 0.15846
266 ->285 0.15829
267 ->275 -0.17313
267 ->278 0.13129
267 ->286 0.15089
268 ->274 0.17304

268 ->279 0.13122
268 ->287 0.15080
269 ->276 -0.15090
269 ->280 0.15743
269 ->284 0.12862
270 ->283 0.20458
271 ->282 -0.20469
272 ->281 0.22928
273 ->280 0.13473
273 ->284 -0.15862

Excited State 24: Singlet-A 2.1522 eV 576.08 nm f=0.0000 <S**2>=0.000
265 ->281 0.11760
266 ->276 -0.15066
266 ->280 0.15224
266 ->284 0.13463
267 ->275 0.17004
267 ->278 -0.13031
267 ->286 -0.15285
268 ->274 0.17013
268 ->279 0.13038
268 ->287 0.15293
269 ->277 0.15788
269 ->285 0.15746
270 ->282 -0.13131
270 ->283 0.18588
271 ->282 0.18576
271 ->283 0.13136
272 ->280 0.15175
272 ->284 -0.17141
273 ->281 0.20783

Excited State 25: Singlet-E 2.1528 eV 575.93 nm f=0.0014 <S**2>=0.000
266 ->274 0.13646
266 ->275 -0.10749
266 ->279 0.14635
266 ->286 0.13660
267 ->276 0.12140
267 ->277 0.12884
267 ->280 -0.12676
267 ->284 -0.10483
267 ->285 0.12879
269 ->275 0.17000
269 ->278 -0.15278
269 ->286 -0.11007

270 ->280 0.10962
270 ->284 -0.17296
271 ->281 0.21935
272 ->282 -0.19309
272 ->283 0.10748
273 ->282 0.16037
273 ->283 0.12688

Excited State 26: Singlet-E 2.1528 eV 575.93 nm f=0.0014 <S**2>=0.000
266 ->274 0.10749
266 ->275 0.13646
266 ->278 -0.14635
266 ->287 0.13660
268 ->276 -0.12140
268 ->277 0.12884
268 ->280 0.12676
268 ->284 0.10483
268 ->285 0.12879
269 ->274 0.17000
269 ->279 0.15278
269 ->287 0.11007
270 ->281 0.21935
271 ->280 0.10962
271 ->284 -0.17296
272 ->282 0.10748
272 ->283 0.19309
273 ->282 -0.12688
273 ->283 0.16037

Excited state symmetry could not be determined.
Excited State 27: Singlet-?Sym 2.2523 eV 550.47 nm f=0.0157 <S**2>=0.000
254 ->274 -0.10678
254 ->275 -0.16185
255 ->274 0.16185
255 ->275 -0.10678
257 ->274 -0.10870
257 ->275 -0.11765
258 ->274 0.11765
258 ->275 -0.10869
260 ->276 -0.12326
262 ->274 0.20631
262 ->275 -0.24344
263 ->274 0.24344
263 ->275 0.20631
273 ->276 0.11560

Excited State 28: Singlet-E 2.2623 eV 548.06 nm f=0.0121 <S**2>=0.000
256 ->274 -0.14614
259 ->274 -0.15154
260 ->274 -0.13029
260 ->275 -0.15782
264 ->274 0.49143
264 ->275 -0.15387

Excited State 29: Singlet-E 2.2623 eV 548.06 nm f=0.0121 <S**2>=0.000
256 ->275 -0.14614
259 ->275 -0.15154
260 ->274 -0.15782
260 ->275 0.13029
264 ->274 0.15387
264 ->275 0.49143

Excited state symmetry could not be determined.
Excited State 30: Singlet-?Sym 2.2655 eV 547.26 nm f=0.0000 <S**2>=0.000
254 ->274 -0.20764
255 ->275 0.20765
256 ->276 -0.10592
257 ->274 -0.16871
258 ->275 0.16871
259 ->276 -0.10659
260 ->277 0.11428
262 ->275 0.26127
263 ->274 0.26127

Excited State 31: Singlet-E 2.3107 eV 536.57 nm f=0.0389 <S**2>=0.000
253 ->275 -0.11292
256 ->274 -0.10069
256 ->275 0.14625
259 ->275 0.14645
260 ->275 -0.20995
264 ->274 -0.26521
264 ->275 0.36718
266 ->282 0.11390
267 ->281 -0.11020
269 ->282 -0.10617

Excited State 32: Singlet-E 2.3107 eV 536.57 nm f=0.0389 <S**2>=0.000
253 ->274 0.11292
256 ->274 0.14625
256 ->275 0.10069

259 ->274 0.14645
260 ->274 0.20995
264 ->274 0.36718
264 ->275 0.26521
266 ->283 0.11390
268 ->281 0.11020
269 ->283 0.10617

Excited state symmetry could not be determined.
Excited State 33: Singlet-?Sym 2.3245 eV 533.38 nm f=0.0095 <S**2>=0.000
254 ->275 0.13954
255 ->274 -0.13954
262 ->274 0.28747
262 ->275 -0.22455
263 ->274 0.22455
263 ->275 0.28747
266 ->281 0.13269
267 ->282 -0.13115
268 ->283 0.13115
273 ->276 -0.10823

Excited state symmetry could not be determined.
Excited State 34: Singlet-?Sym 2.3485 eV 527.93 nm f=0.0000 <S**2>=0.000
254 ->274 0.11194
255 ->275 -0.11194
262 ->274 0.21851
262 ->275 0.36268
263 ->274 0.36269
263 ->275 -0.21851

Excited state symmetry could not be determined.
Excited State 35: Singlet-?Sym 2.3827 eV 520.35 nm f=0.0000 <S**2>=0.000
262 ->274 0.44770
262 ->275 -0.18883
263 ->274 -0.18884
263 ->275 -0.44769

Excited state symmetry could not be determined.
Excited State 36: Singlet-?Sym 2.3833 eV 520.22 nm f=0.0014 <S**2>=0.000
262 ->274 0.34454
262 ->275 0.35544
263 ->274 -0.35543
263 ->275 0.34454

Excited State 37: Singlet-B 2.5445 eV 487.26 nm f=0.0002 <S**2>=0.000

254 ->283 0.12446
255 ->282 0.12450
256 ->281 0.13710
257 ->283 0.10490
258 ->282 0.10493
259 ->281 0.13567
260 ->280 0.11465
260 ->284 -0.12411
266 ->277 -0.11809
269 ->276 0.24583
269 ->284 -0.10350
270 ->283 0.18020
271 ->282 -0.18026
272 ->281 0.19803
273 ->280 0.11324
273 ->284 -0.11832

Excited State 38: Singlet-E 2.5449 eV 487.19 nm f=0.0004 <S**2>=0.000
254 ->284 0.10876
255 ->281 0.15176
256 ->282 0.11971
258 ->281 0.11730
259 ->282 0.11852
260 ->282 -0.13000
260 ->283 -0.10837
265 ->282 -0.10424
266 ->279 0.11051
267 ->276 0.20353
268 ->276 -0.13557
269 ->278 -0.11745
270 ->280 -0.12402
270 ->284 0.12813
271 ->281 -0.19762
272 ->282 0.17261
273 ->282 -0.12552
273 ->283 -0.10534

Excited State 39: Singlet-E 2.5449 eV 487.19 nm f=0.0004 <S**2>=0.000
254 ->281 0.15176
255 ->284 0.10876
256 ->283 0.11971
257 ->281 0.11730
259 ->283 0.11852
260 ->282 -0.10837
260 ->283 0.13000

265 ->283 0.10424
266 ->278 0.11051
267 ->276 0.13557
268 ->276 0.20353
269 ->279 -0.11745
270 ->281 0.19762
271 ->280 0.12402
271 ->284 -0.12813
272 ->283 0.17262
273 ->282 -0.10534
273 ->283 0.12552

Excited State 40: Singlet-A 2.5451 eV 487.15 nm f=0.0000 <S**2>=0.000
254 ->282 -0.10819
254 ->283 0.10655
255 ->282 -0.10651
255 ->283 -0.10822
256 ->284 -0.10288
260 ->281 0.16996
265 ->281 0.13674
266 ->276 0.24530
269 ->277 -0.11860
270 ->282 -0.11382
270 ->283 0.16056
271 ->282 0.16050
271 ->283 0.11385
272 ->280 0.13490
272 ->284 -0.14467
273 ->281 0.16452

Excited State 41: Singlet-B 2.6247 eV 472.38 nm f=0.0498 <S**2>=0.000
254 ->274 0.10336
254 ->275 0.14919
255 ->274 -0.14919
255 ->275 0.10336
266 ->281 -0.12550
267 ->282 0.12407
268 ->283 -0.12407
273 ->276 0.56847

Excited State 42: Singlet-E 2.6743 eV 463.61 nm f=0.0593 <S**2>=0.000
252 ->274 0.15225
253 ->274 -0.16286
256 ->275 -0.17596
259 ->274 -0.10092

261 ->274 0.23766
261 ->275 0.51303
270 ->276 0.12398

Excited State 43: Singlet-E 2.6743 eV 463.61 nm f=0.0593 <S**2>=0.000
252 ->275 -0.15225
253 ->275 0.16286
256 ->274 0.17596
259 ->275 -0.10092
261 ->274 0.51303
261 ->275 -0.23766
271 ->276 0.12398

Excited state symmetry could not be determined.
Excited State 44: Singlet-?Sym 2.7101 eV 457.49 nm f=0.0000 <S**2>=0.000
254 ->274 -0.20601
254 ->275 -0.21561
255 ->274 -0.21524
255 ->275 0.20731
257 ->274 0.20742
257 ->275 0.33565
258 ->274 0.33487
258 ->275 -0.20905

Excited state symmetry could not be determined.
Excited State 45: Singlet-?Sym 2.7104 eV 457.44 nm f=0.0000 <S**2>=0.000
254 ->274 -0.28550
255 ->275 -0.28455
257 ->274 0.35873
257 ->275 -0.16900
258 ->274 0.17053
258 ->275 0.35778

Excited State 46: Singlet-E 2.7173 eV 456.27 nm f=0.0147 <S**2>=0.000
253 ->275 -0.17632
259 ->274 0.26668
259 ->275 -0.23557
260 ->274 0.13960
260 ->275 0.31544
270 ->276 0.31481

Excited State 47: Singlet-E 2.7173 eV 456.27 nm f=0.0147 <S**2>=0.000
253 ->274 -0.17631
259 ->274 0.23557
259 ->275 0.26668

260 ->274 0.31544
260 ->275 -0.13960
271 ->276 0.31481

Excited State 48: Singlet-A 2.7205 eV 455.74 nm f=0.0000 <S**2>=0.000
254 ->274 0.18990
255 ->275 -0.18990
257 ->274 0.16497
258 ->275 -0.16497
266 ->280 -0.10809
266 ->284 0.11895
267 ->282 -0.16001
268 ->283 -0.16001
269 ->281 -0.16091
272 ->276 0.45977

Excited State 49: Singlet-E 2.7416 eV 452.23 nm f=0.0324 <S**2>=0.000
252 ->274 -0.15576
252 ->275 0.10712
253 ->274 0.25508
253 ->275 0.25744
256 ->274 0.30405
256 ->275 -0.18521
259 ->275 0.13959
261 ->274 -0.20160
270 ->276 0.26522

Excited State 50: Singlet-E 2.7416 eV 452.23 nm f=0.0324 <S**2>=0.000
252 ->274 0.10712
252 ->275 0.15576
253 ->274 0.25744
253 ->275 -0.25508
256 ->274 0.18521
256 ->275 0.30405
259 ->274 -0.13959
261 ->275 0.20160
271 ->276 0.26522

Excited State 51: Singlet-E 2.7980 eV 443.12 nm f=0.0046 <S**2>=0.000
251 ->275 0.19690
253 ->275 0.27663
256 ->274 -0.18521
256 ->275 0.32492
259 ->275 0.28997
260 ->274 -0.17613

260 ->275 0.31506

Excited State 52: Singlet-E 2.7980 eV 443.12 nm f=0.0046 <S**2>=0.000
251 ->274 -0.19690
253 ->274 -0.27663
256 ->274 0.32492
256 ->275 0.18521
259 ->274 0.28997
260 ->274 -0.31506
260 ->275 -0.17613

Excited state symmetry could not be determined.
Excited State 53: Singlet-?Sym 2.7993 eV 442.90 nm f=0.0000 <S**2>=0.000
254 ->274 0.33831
254 ->275 -0.18794
255 ->274 0.18797
255 ->275 0.33830
257 ->274 0.19786
257 ->275 -0.24227
258 ->274 0.24229
258 ->275 0.19786

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 2.7999 eV 442.82 nm f=0.0000 <S**2>=0.000
254 ->274 0.17957
254 ->275 0.34898
255 ->274 0.34897
255 ->275 -0.17960
257 ->275 0.30208
258 ->274 0.30206

Excited State 55: Singlet-E 2.8083 eV 441.49 nm f=0.0196 <S**2>=0.000
251 ->274 0.20210
251 ->275 -0.21444
253 ->274 0.13540
253 ->275 -0.22161
256 ->275 -0.19621
259 ->274 0.23685
259 ->275 0.31305
260 ->274 -0.29392
261 ->274 0.18201

Excited State 56: Singlet-E 2.8083 eV 441.49 nm f=0.0196 <S**2>=0.000
251 ->274 0.21444
251 ->275 0.20210

253 ->274 0.22161
253 ->275 0.13540
256 ->274 -0.19621
259 ->274 0.31305
259 ->275 -0.23685
260 ->275 -0.29392
261 ->275 0.18201

Excited state symmetry could not be determined.
Excited State 57: Singlet-?Sym 2.8136 eV 440.66 nm f=0.0005 <S**2>=0.000
254 ->275 0.29666
255 ->274 -0.29666
257 ->274 -0.20029
257 ->275 -0.34390
258 ->274 0.34390
258 ->275 -0.20028

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 2.8143 eV 440.54 nm f=0.0000 <S**2>=0.000
254 ->274 0.21217
254 ->275 -0.22710
255 ->274 -0.22709
255 ->275 -0.21217
257 ->274 -0.33872
257 ->275 0.19452
258 ->274 0.19452
258 ->275 0.33872

Excited State 59: Singlet-E 2.8471 eV 435.48 nm f=0.0006 <S**2>=0.000
247 ->274 -0.12954
247 ->275 0.11759
251 ->274 -0.36715
251 ->275 0.38318
252 ->274 0.11858
253 ->274 0.19395
253 ->275 -0.21157
256 ->275 -0.20121
261 ->274 0.12134

Excited State 60: Singlet-E 2.8471 eV 435.48 nm f=0.0006 <S**2>=0.000
247 ->274 0.11759
247 ->275 0.12954
251 ->274 0.38318
251 ->275 0.36715
252 ->275 -0.11858

253 ->274 -0.21157
253 ->275 -0.19395
256 ->274 0.20121
261 ->275 -0.12134

Excited State 61: Singlet-B 2.8651 eV 432.74 nm f=0.0196 <S**2>=0.000
254 ->274 -0.12946
254 ->275 -0.19824
255 ->274 0.19824
255 ->275 -0.12946
265 ->276 -0.11802
266 ->281 0.12095
267 ->282 -0.11923
268 ->283 0.11923
270 ->278 -0.11453
270 ->287 0.10567
271 ->279 0.11453
271 ->286 0.10567
272 ->277 0.13757
272 ->285 0.12181
273 ->276 0.28591
273 ->280 0.11719
273 ->284 0.11976

Excited State 62: Singlet-B 2.9062 eV 426.62 nm f=0.0002 <S**2>=0.000
266 ->285 0.10376
267 ->286 0.10404
268 ->287 0.10404
269 ->276 0.60661
269 ->280 0.10001

Excited State 63: Singlet-E 2.9080 eV 426.35 nm f=0.0013 <S**2>=0.000
267 ->276 0.54590
268 ->276 -0.26031

Excited State 64: Singlet-E 2.9080 eV 426.35 nm f=0.0013 <S**2>=0.000
267 ->276 0.26031
268 ->276 0.54590

Excited State 65: Singlet-A 2.9084 eV 426.30 nm f=0.0000 <S**2>=0.000
266 ->276 0.61150
267 ->286 -0.10524
268 ->287 0.10525
269 ->285 0.10495

Excited State 66: Singlet-A 2.9269 eV 423.60 nm f=0.0000 <S**2>=0.000
254 ->274 -0.15661
255 ->275 0.15661
257 ->274 -0.12120
258 ->275 0.12120
270 ->279 0.11151
271 ->278 -0.11151
272 ->276 0.46306
272 ->280 0.11195
272 ->284 0.10697
273 ->277 0.14038
273 ->285 0.11986

Excited State 67: Singlet-E 2.9321 eV 422.86 nm f=0.0053 <S**2>=0.000
256 ->274 -0.13397
259 ->274 -0.14547
260 ->274 -0.10197
260 ->275 -0.14346
270 ->276 0.46219
270 ->280 0.10593
270 ->284 0.10175
271 ->277 0.10654
271 ->285 0.10219
272 ->279 0.11080
273 ->278 -0.11524
273 ->287 0.10175

Excited State 68: Singlet-E 2.9321 eV 422.86 nm f=0.0053 <S**2>=0.000
256 ->275 -0.13397
259 ->275 -0.14547
260 ->274 -0.14346
260 ->275 0.10197
270 ->277 0.10654
270 ->285 0.10219
271 ->276 0.46219
271 ->280 0.10593
271 ->284 0.10175
272 ->278 -0.11080
273 ->279 0.11524
273 ->286 0.10175

Excited State 69: Singlet-B 3.1079 eV 398.93 nm f=0.0009 <S**2>=0.000
248 ->275 0.31522
249 ->274 -0.31521
265 ->276 0.48561

Excited state symmetry could not be determined.
Excited State 70: Singlet-?Sym 3.1143 eV 398.11 nm f=0.0000 <S**2>=0.000
248 ->274 -0.30028
248 ->275 0.38279
249 ->274 0.38280
249 ->275 0.30027

Excited State 71: Singlet-E 3.1146 eV 398.07 nm f=0.0106 <S**2>=0.000
247 ->274 0.16940
247 ->275 -0.35120
250 ->275 0.54369
251 ->275 0.12563

Excited State 72: Singlet-E 3.1146 eV 398.07 nm f=0.0106 <S**2>=0.000
247 ->274 0.35120
247 ->275 0.16940
250 ->274 0.54369
251 ->274 -0.12563

Excited State 73: Singlet-B 3.1209 eV 397.27 nm f=0.0222 <S**2>=0.000
248 ->275 -0.36420
249 ->274 0.36420
265 ->276 0.45810

Excited state symmetry could not be determined.
Excited State 74: Singlet-?Sym 3.1863 eV 389.12 nm f=0.0020 <S**2>=0.000
241 ->274 0.23737
242 ->275 0.23738
245 ->274 0.36867
245 ->275 -0.18474
246 ->274 0.18474
246 ->275 0.36867
251 ->276 0.12116

Excited state symmetry could not be determined.
Excited State 75: Singlet-?Sym 3.1942 eV 388.15 nm f=0.0000 <S**2>=0.000
241 ->274 0.11800
241 ->275 0.17396
242 ->274 0.17396
242 ->275 -0.11799
245 ->274 0.16724
245 ->275 0.40096
246 ->274 0.40096
246 ->275 -0.16723

Excited state symmetry could not be determined.
Excited State 76: Singlet-?Sym 3.2257 eV 384.36 nm f=0.0007 <S**2>=0.000
248 ->274 0.48936
249 ->275 0.48935

Excited state symmetry could not be determined.
Excited State 77: Singlet-?Sym 3.2294 eV 383.92 nm f=0.0000 <S**2>=0.000
248 ->274 -0.38849
248 ->275 -0.30142
249 ->274 -0.30142
249 ->275 0.38849

Excited State 78: Singlet-E 3.2325 eV 383.55 nm f=0.0198 <S**2>=0.000
243 ->274 -0.11007
247 ->274 -0.33053
247 ->275 -0.37804
250 ->274 0.39405
250 ->275 -0.10644
251 ->274 0.10585
251 ->275 0.12708

Excited State 79: Singlet-E 3.2325 eV 383.55 nm f=0.0198 <S**2>=0.000
243 ->275 0.11007
247 ->274 -0.37804
247 ->275 0.33053
250 ->274 0.10644
250 ->275 0.39405
251 ->274 0.12708
251 ->275 -0.10585

Excited State 80: Singlet-E 3.2457 eV 381.99 nm f=0.0438 <S**2>=0.000
243 ->274 0.11988
243 ->275 0.39303
244 ->274 0.33909
244 ->275 -0.29031
247 ->274 0.12274
250 ->275 -0.11182
252 ->274 -0.10075
252 ->275 -0.16922

Excited State 81: Singlet-E 3.2457 eV 381.99 nm f=0.0438 <S**2>=0.000
243 ->274 0.39303
243 ->275 -0.11988
244 ->274 0.29031

244 ->275 0.33909
247 ->275 -0.12274
250 ->274 0.11182
252 ->274 -0.16922
252 ->275 0.10075

Excited state symmetry could not be determined.
Excited State 82: Singlet-?Sym 3.2815 eV 377.82 nm f=0.0015 <S**2>=0.000
241 ->274 -0.21681
241 ->275 -0.26217
242 ->274 0.26217
242 ->275 -0.21681
245 ->275 -0.34435
246 ->274 0.34435

Excited state symmetry could not be determined.
Excited State 83: Singlet-?Sym 3.3010 eV 375.59 nm f=0.0000 <S**2>=0.000
241 ->274 -0.22657
241 ->275 0.24508
242 ->274 0.24508
242 ->275 0.22657
245 ->274 -0.34727
245 ->275 0.11519
246 ->274 0.11518
246 ->275 0.34727

Excited State 84: Singlet-E 3.3171 eV 373.77 nm f=0.8130 <S**2>=0.000
244 ->275 -0.21640
252 ->275 0.53150
253 ->274 -0.14915
261 ->274 0.16378
262 ->276 0.15794
263 ->276 0.11214

Excited State 85: Singlet-E 3.3171 eV 373.77 nm f=0.8130 <S**2>=0.000
244 ->274 0.21640
252 ->274 0.53150
253 ->275 0.14915
261 ->275 -0.16378
262 ->276 0.11214
263 ->276 -0.15794

Excited state symmetry could not be determined.
Excited State 86: Singlet-?Sym 3.3390 eV 371.32 nm f=0.0000 <S**2>=0.000
241 ->274 0.30631

241 ->275 0.31682
242 ->274 0.31679
242 ->275 -0.30635
245 ->275 -0.18647
246 ->274 -0.18648

Excited state symmetry could not be determined.
Excited State 87: Singlet-?Sym 3.3406 eV 371.15 nm f=0.0004 <S**2>=0.000
241 ->274 0.34668
241 ->275 -0.21804
242 ->274 0.21808
242 ->275 0.34665
245 ->274 -0.24027
246 ->275 -0.24027

Excited State 88: Singlet-E 3.4116 eV 363.42 nm f=0.0139 <S**2>=0.000
243 ->275 0.50434
244 ->274 -0.30661
244 ->275 0.34045

Excited State 89: Singlet-E 3.4116 eV 363.42 nm f=0.0139 <S**2>=0.000
243 ->274 0.50434
244 ->274 -0.34045
244 ->275 -0.30661

Excited State 90: Singlet-A 3.4248 eV 362.02 nm f=0.0000 <S**2>=0.000
256 ->276 -0.11470
259 ->276 -0.11286
260 ->277 0.10255
264 ->276 0.46928
267 ->282 0.11921
268 ->283 0.11921
269 ->281 0.11986
270 ->279 0.10016
271 ->278 -0.10016
273 ->277 0.10145

Excited State 91: Singlet-E 3.4512 eV 359.25 nm f=0.0738 <S**2>=0.000
252 ->275 -0.13632
254 ->277 0.10521
255 ->276 0.14208
258 ->276 0.10094
260 ->279 0.11889
262 ->276 0.14499
263 ->276 0.25810

266 ->283 0.13072
268 ->281 0.12556
269 ->283 0.11995
270 ->277 0.13270
272 ->278 -0.10182
273 ->279 0.11326

Excited State 92: Singlet-E 3.4512 eV 359.25 nm f=0.0738 <S**2>=0.000
252 ->274 -0.13632
254 ->276 0.14208
255 ->277 0.10521
257 ->276 0.10094
260 ->278 0.11889
262 ->276 0.25810
263 ->276 -0.14499
266 ->282 0.13072
267 ->281 -0.12556
269 ->282 -0.11995
271 ->277 -0.13270
272 ->279 -0.10182
273 ->278 0.11326

Excited state symmetry could not be determined.
Excited State 93: Singlet-?Sym 3.4565 eV 358.70 nm f=0.0000 <S**2>=0.000
241 ->275 -0.35236
242 ->274 0.35236
245 ->274 0.18619
245 ->275 0.28614
246 ->274 -0.28614
246 ->275 0.18619

Excited state symmetry could not be determined.
Excited State 94: Singlet-?Sym 3.4609 eV 358.25 nm f=0.0000 <S**2>=0.000
241 ->274 0.29049
241 ->275 -0.22462
242 ->274 -0.22462
242 ->275 -0.29049
245 ->274 -0.30622
245 ->275 0.13779
246 ->274 0.13778
246 ->275 0.30622

Excited State 95: Singlet-B 3.4870 eV 355.56 nm f=0.0002 <S**2>=0.000
254 ->278 0.11821
255 ->279 0.11821

256 ->277 -0.11048
259 ->277 -0.10910
260 ->276 0.20743
260 ->280 -0.12321
260 ->284 -0.10459
261 ->276 0.10318
265 ->276 -0.14185
266 ->281 -0.14920
267 ->282 0.14672
268 ->283 -0.14672
269 ->280 -0.10992
269 ->284 0.10088
270 ->278 0.11452
271 ->279 -0.11452
272 ->277 -0.14224

Excited State 96: Singlet-A 3.5432 eV 349.92 nm f=0.0000 <S**2>=0.000
256 ->276 0.13226
259 ->276 0.12818
264 ->276 0.51616

Excited State 97: Singlet-E 3.5487 eV 349.38 nm f=0.0003 <S**2>=0.000
243 ->274 -0.12148
254 ->281 0.18853
255 ->280 -0.12294
255 ->284 0.13743
256 ->283 0.14265
257 ->281 0.14520
258 ->284 0.10134
259 ->283 0.14253
260 ->282 -0.14504
260 ->283 0.15461
266 ->278 -0.13143
268 ->277 0.11686
269 ->279 0.13843
270 ->281 -0.15374
271 ->280 -0.10111
271 ->284 0.10235
272 ->283 -0.13439
273 ->282 0.12783
273 ->283 -0.13485

Excited State 98: Singlet-E 3.5487 eV 349.38 nm f=0.0003 <S**2>=0.000
243 ->275 0.12148
254 ->280 -0.12295

254 ->284 0.13743
255 ->281 0.18853
256 ->282 0.14265
257 ->284 0.10133
258 ->281 0.14520
259 ->282 0.14253
260 ->282 -0.15461
260 ->283 -0.14504
266 ->279 -0.13143
267 ->277 -0.11686
269 ->278 0.13843
270 ->280 0.10111
270 ->284 -0.10235
271 ->281 0.15374
272 ->282 -0.13439
273 ->282 0.13485
273 ->283 0.12783

Excited State 99: Singlet-B 3.5506 eV 349.19 nm f=0.0000 <S**2>=0.000
245 ->274 -0.10207
246 ->275 -0.10216
254 ->282 0.10721
254 ->283 0.15238
255 ->282 0.15266
255 ->283 -0.10693
256 ->281 0.16816
257 ->283 0.12994
258 ->282 0.13019
259 ->281 0.16795
260 ->280 0.13878
260 ->284 -0.15849
266 ->277 0.14936
266 ->285 0.10369
267 ->278 0.11678
267 ->286 0.10114
268 ->279 0.11654
268 ->287 0.10092
269 ->280 0.10017
269 ->284 0.10865
270 ->283 -0.13936
271 ->282 0.13962
272 ->281 -0.15886
273 ->280 -0.13306
273 ->284 0.12903

Excited State 100: Singlet-A 3.5506 eV 349.19 nm f=0.0000 <S**2>=0.000

245 ->275	-0.11119
246 ->274	-0.11132
254 ->282	-0.13227
254 ->283	0.13062
255 ->282	-0.13029
255 ->283	-0.13250
256 ->280	0.10731
256 ->284	-0.12916
257 ->283	0.11658
258 ->282	-0.11630
259 ->280	0.10800
259 ->284	-0.12812
260 ->281	0.21030
266 ->280	0.10243
266 ->284	0.10598
267 ->278	-0.11322
267 ->286	-0.10008
268 ->279	0.11347
268 ->287	0.10030
269 ->277	0.14902
269 ->285	0.10324
270 ->283	-0.12306
271 ->282	-0.12276
272 ->280	-0.11296
272 ->284	0.11124
273 ->281	-0.18466

Table S7: Vertical Excitation energies of $TAP^{Fc}Mg$ using PBE1PBE PCM-TDDFT

Excited State 1: Singlet-E 2.0453 eV 606.20 nm f=0.1970 <S**2>=0.000

241 ->251	0.12728
241 ->255	-0.11360
242 ->258	0.11322
244 ->256	0.10420
245 ->259	-0.10217
246 ->253	0.12531
246 ->260	0.10886
247 ->252	-0.11373
247 ->253	0.15126
247 ->260	-0.13473
248 ->250	-0.23859
248 ->251	0.11595
248 ->254	0.12351
248 ->255	0.14438
249 ->250	0.25155
249 ->251	0.29754

This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3087.10571279
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-E 2.0453 eV 606.20 nm f=0.1970 <S**2>=0.000

241 ->250	0.12728
241 ->254	-0.11360
242 ->259	0.11322
243 ->256	0.10420
245 ->258	-0.10217
246 ->252	-0.11373
246 ->253	-0.15126
246 ->260	-0.13473
247 ->253	0.12531
247 ->260	-0.10886
248 ->250	-0.11595
248 ->251	-0.23859
248 ->254	-0.14438
248 ->255	0.12351
249 ->250	0.29754
249 ->251	-0.25155

Excited state symmetry could not be determined.

Excited State 3: Singlet-?Sym 2.0718 eV 598.43 nm f=0.0022 <S**2>=0.000

241 ->256	-0.10503
242 ->253	-0.20740

243 ->250 0.11491
243 ->251 -0.25370
243 ->254 -0.19917
244 ->250 0.25370
244 ->251 0.11491
244 ->255 -0.19917
245 ->252 -0.16201
245 ->260 -0.19089
246 ->251 -0.12717
246 ->259 -0.11515
247 ->250 0.12717
247 ->258 0.11515
248 ->257 -0.12897

Excited state symmetry could not be determined.
Excited State 4: Singlet-?Sym 2.0728 eV 598.14 nm f=0.0000 <S**2>=0.000
241 ->257 0.10728
242 ->252 0.16595
242 ->260 0.19456
243 ->251 0.29954
243 ->254 0.21245
244 ->250 0.29954
244 ->255 -0.21245
245 ->253 0.22732
246 ->259 0.12751
247 ->258 0.12751
248 ->256 0.13948
249 ->257 0.10121

Excited State 5: Singlet-E 2.0729 eV 598.11 nm f=0.0015 <S**2>=0.000
242 ->250 0.27285
242 ->251 0.13712
242 ->255 -0.21134
244 ->252 0.15521
244 ->253 -0.22453
244 ->260 0.18121
245 ->250 -0.30180
245 ->255 0.20965
247 ->256 0.13613
247 ->257 -0.13765
248 ->258 0.11333

Excited State 6: Singlet-E 2.0729 eV 598.11 nm f=0.0015 <S**2>=0.000
242 ->250 -0.13712
242 ->251 0.27285

242 ->254 0.21134
243 ->252 0.15521
243 ->253 0.22453
243 ->260 0.18121
245 ->251 0.30180
245 ->254 0.20965
246 ->256 0.13613
246 ->257 0.13765
248 ->259 0.11333

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 2.0829 eV 595.26 nm f=0.0112 <S**2>=0.000
241 ->252 -0.11424
241 ->260 -0.15102
242 ->257 0.13183
243 ->251 0.12889
243 ->259 0.10587
244 ->250 -0.12889
244 ->258 -0.10587
245 ->256 0.14000
246 ->251 -0.26897
246 ->254 -0.19439
247 ->250 0.26897
247 ->255 -0.19439
248 ->253 -0.19764
249 ->252 -0.10661
249 ->260 -0.12591

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 2.0966 eV 591.36 nm f=0.0000 <S**2>=0.000
241 ->253 0.17924
242 ->256 -0.14815
243 ->259 -0.14061
244 ->258 -0.14061
245 ->257 -0.14973
246 ->251 0.27803
246 ->254 0.21117
247 ->250 0.27803
247 ->255 -0.21117
248 ->252 0.14857
248 ->260 0.19360
249 ->253 0.14787

Excited State 9: Singlet-E 2.3066 eV 537.52 nm f=0.2557 <S**2>=0.000
242 ->258 -0.11475

244 ->256 -0.11428
248 ->250 0.23845
249 ->250 0.45097
249 ->251 0.31631

Excited State 10: Singlet-E 2.3066 eV 537.52 nm f=0.2557 <S**2>=0.000
242 ->259 0.11475
243 ->256 0.11428
248 ->251 -0.23845
249 ->250 -0.31631
249 ->251 0.45097

Excited State 11: Singlet-E 2.4653 eV 502.91 nm f=0.0393 <S**2>=0.000
235 ->254 0.10037
242 ->250 -0.10080
242 ->258 0.12478
242 ->259 -0.17342
243 ->256 -0.19725
243 ->257 -0.21808
245 ->259 -0.21340
248 ->250 0.17120
248 ->251 -0.43022

Excited State 12: Singlet-E 2.4653 eV 502.91 nm f=0.0393 <S**2>=0.000
235 ->255 0.10037
242 ->251 -0.10080
242 ->258 0.17342
242 ->259 0.12478
244 ->256 0.19725
244 ->257 -0.21808
245 ->258 -0.21340
248 ->250 0.43022
248 ->251 0.17120

Excited State 13: Singlet-B 2.4693 eV 502.09 nm f=0.0125 <S**2>=0.000
233 ->255 0.12065
234 ->254 -0.12065
235 ->253 -0.12460
242 ->257 0.25669
243 ->258 -0.13466
243 ->259 0.21575
244 ->258 -0.21575
244 ->259 -0.13466
245 ->256 0.25536
246 ->251 0.25649

247 ->250 -0.25649

Excited state symmetry could not be determined.
Excited State 14: Singlet-?Sym 2.4778 eV 500.39 nm f=0.0000 <S**2>=0.000
233 ->255 0.10091
234 ->254 0.10091
242 ->256 -0.21171
243 ->259 -0.20281
244 ->258 -0.20281
245 ->257 -0.19623
246 ->250 0.27395
246 ->251 -0.16372
247 ->250 -0.16372
247 ->251 -0.27395

Excited state symmetry could not be determined.
Excited State 15: Singlet-?Sym 2.4849 eV 498.96 nm f=0.0000 <S**2>=0.000
241 ->256 0.17162
243 ->251 -0.19714
244 ->250 0.19714
246 ->250 0.28577
246 ->259 0.19323
247 ->251 0.28577
247 ->258 -0.19323
248 ->257 0.21067
249 ->256 0.14358

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 2.4874 eV 498.46 nm f=0.0000 <S**2>=0.000
241 ->257 -0.13074
242 ->256 -0.13491
243 ->251 0.20809
243 ->259 -0.13199
244 ->250 0.20809
244 ->258 -0.13199
245 ->257 -0.16415
246 ->250 -0.17384
246 ->251 -0.16674
246 ->259 -0.17510
247 ->250 -0.16674
247 ->251 0.17384
247 ->258 -0.17510
248 ->256 -0.18776
249 ->257 -0.11826

Excited State 17: Singlet-E 2.4979 eV 496.36 nm f=0.0001 <S**2>=0.000
233 ->256 -0.10183
241 ->258 -0.19607
242 ->250 -0.20840
242 ->251 -0.12018
245 ->250 0.29154
247 ->256 0.23836
247 ->257 -0.24368
248 ->258 0.19542
248 ->259 0.14387
249 ->258 -0.16416

Excited State 18: Singlet-E 2.4979 eV 496.36 nm f=0.0001 <S**2>=0.000
234 ->256 -0.10183
241 ->259 -0.19607
242 ->250 -0.12018
242 ->251 0.20840
245 ->251 0.29154
246 ->256 -0.23836
246 ->257 -0.24368
248 ->258 0.14387
248 ->259 -0.19542
249 ->259 -0.16416

Excited state symmetry could not be determined.
Excited State 19: Singlet-?Sym 2.5181 eV 492.38 nm f=0.0000 <S**2>=0.000
241 ->257 -0.13424
243 ->251 0.14940
244 ->250 0.14940
246 ->250 0.36791
246 ->251 0.12207
246 ->259 -0.14341
247 ->250 0.12207
247 ->251 -0.36791
247 ->258 -0.14341
248 ->256 -0.15418
249 ->257 -0.10917

Excited state symmetry could not be determined.
Excited State 20: Singlet-?Sym 2.5257 eV 490.90 nm f=0.0001 <S**2>=0.000
241 ->256 -0.11793
243 ->251 0.15585
244 ->250 -0.15585
246 ->250 0.39317
246 ->259 -0.13295

247 ->251 0.39317
247 ->258 0.13295
248 ->257 -0.14336

Excited State 21: Singlet-E 2.5954 eV 477.70 nm f=0.0496 <S**2>=0.000
241 ->251 0.19786
242 ->250 0.34932
242 ->251 0.14803
245 ->250 0.34613
248 ->250 0.17163
248 ->251 -0.19889

Excited State 22: Singlet-E 2.5954 eV 477.70 nm f=0.0496 <S**2>=0.000
241 ->250 -0.19786
242 ->250 0.14803
242 ->251 -0.34932
245 ->251 0.34613
248 ->250 -0.19889
248 ->251 -0.17163

Excited state symmetry could not be determined.
Excited State 23: Singlet-?Sym 2.6108 eV 474.88 nm f=0.0000 <S**2>=0.000
243 ->250 -0.48819
244 ->251 0.48819

Excited state symmetry could not be determined.
Excited State 24: Singlet-?Sym 2.6118 eV 474.70 nm f=0.0000 <S**2>=0.000
243 ->250 0.45899
243 ->251 0.18045
244 ->250 -0.18045
244 ->251 0.45899

Excited State 25: Singlet-E 2.6295 eV 471.51 nm f=0.1047 <S**2>=0.000
233 ->253 -0.10771
241 ->250 -0.18346
241 ->251 -0.12005
242 ->250 0.24250
242 ->251 0.22519
245 ->250 0.31192
245 ->251 -0.13806
248 ->250 -0.21144

Excited State 26: Singlet-E 2.6295 eV 471.51 nm f=0.1047 <S**2>=0.000
234 ->253 0.10771
241 ->250 0.12005

241 ->251 -0.18346
242 ->250 0.22519
242 ->251 -0.24250
245 ->250 0.13806
245 ->251 0.31192
248 ->251 0.21144

Excited state symmetry could not be determined.
Excited State 27: Singlet-?Sym 2.6682 eV 464.67 nm f=0.0105 <S**2>=0.000
232 ->260 -0.13947
233 ->250 -0.12365
233 ->255 0.17493
234 ->251 -0.12365
234 ->254 -0.17493
235 ->253 -0.18106
241 ->260 0.11075
246 ->251 -0.27221
246 ->254 0.17555
247 ->250 0.27221
247 ->255 0.17555
248 ->253 0.17791
249 ->260 0.13418

Excited state symmetry could not be determined.
Excited State 28: Singlet-?Sym 2.6842 eV 461.91 nm f=0.0000 <S**2>=0.000
232 ->253 0.14970
233 ->250 -0.11806
233 ->255 0.16927
234 ->251 0.11806
234 ->254 0.16927
235 ->252 0.10260
235 ->260 0.15818
241 ->253 -0.10938
246 ->251 0.29557
246 ->254 -0.17462
247 ->250 0.29557
247 ->255 0.17462
248 ->260 -0.16924
249 ->253 -0.14690

Excited State 29: Singlet-E 2.7317 eV 453.88 nm f=0.0419 <S**2>=0.000
234 ->253 0.11026
235 ->254 0.10538
241 ->250 -0.25262
241 ->251 0.49753

246 ->253 -0.11125
246 ->260 -0.11095
248 ->254 -0.11202

Excited State 30: Singlet-E 2.7317 eV 453.88 nm f=0.0419 <S**2>=0.000
233 ->253 -0.11026
235 ->255 0.10538
241 ->250 0.49753
241 ->251 0.25262
247 ->253 -0.11125
247 ->260 0.11095
248 ->255 -0.11202

Excited state symmetry could not be determined.
Excited State 31: Singlet-?Sym 2.7643 eV 448.53 nm f=0.0000 <S**2>=0.000
232 ->256 -0.16026
233 ->258 -0.17285
234 ->259 -0.17285
235 ->257 -0.18552
242 ->253 0.20266
243 ->251 -0.25878
243 ->254 0.19906
244 ->250 0.25878
244 ->255 0.19906
245 ->260 0.19589

Excited state symmetry could not be determined.
Excited State 32: Singlet-?Sym 2.7644 eV 448.50 nm f=0.0000 <S**2>=0.000
232 ->257 0.16044
233 ->258 -0.16484
234 ->259 0.16484
235 ->256 0.18526
242 ->260 -0.19774
243 ->251 0.27199
243 ->254 -0.19725
244 ->250 0.27199
244 ->255 0.19725
245 ->253 -0.20007

Excited State 33: Singlet-E 2.7653 eV 448.35 nm f=0.0026 <S**2>=0.000
232 ->258 -0.14094
233 ->256 -0.17953
233 ->257 0.18075
235 ->258 0.16874
241 ->250 0.15119

242 ->250 0.26428
242 ->255 0.19659
244 ->253 0.19491
244 ->260 -0.19215
245 ->250 -0.24831
245 ->255 -0.19248

Excited State 34: Singlet-E 2.7653 eV 448.35 nm f=0.0026 <S**2>=0.000
232 ->259 0.14094
234 ->256 0.17953
234 ->257 0.18075
235 ->259 0.16874
241 ->251 -0.15119
242 ->251 0.26428
242 ->254 -0.19659
243 ->253 -0.19491
243 ->260 -0.19215
245 ->251 0.24831
245 ->254 -0.19248

Excited state symmetry could not be determined.
Excited State 35: Singlet-?Sym 2.9103 eV 426.02 nm f=0.0148 <S**2>=0.000
238 ->250 -0.46547
238 ->251 -0.10414
239 ->250 -0.10414
239 ->251 0.46547

Excited State 36: Singlet-E 2.9119 eV 425.78 nm f=0.0489 <S**2>=0.000
237 ->251 -0.11058
240 ->251 0.66110

Excited State 37: Singlet-E 2.9119 eV 425.78 nm f=0.0489 <S**2>=0.000
237 ->250 0.11058
240 ->250 0.66110

Excited state symmetry could not be determined.
Excited State 38: Singlet-?Sym 2.9384 eV 421.94 nm f=0.0000 <S**2>=0.000
238 ->250 0.39450
238 ->251 0.27551
239 ->250 -0.27551
239 ->251 0.39450

Excited state symmetry could not be determined.
Excited State 39: Singlet-?Sym 3.0600 eV 405.18 nm f=0.0002 <S**2>=0.000
238 ->250 -0.10778

238 ->251 0.48482
239 ->250 0.48482
239 ->251 0.10778

Excited state symmetry could not be determined.
Excited State 40: Singlet-?Sym 3.0684 eV 404.07 nm f=0.0000 <S**2>=0.000
238 ->250 0.27790
238 ->251 -0.40943
239 ->250 0.40943
239 ->251 0.27790

Excited State 41: Singlet-E 3.2551 eV 380.89 nm f=0.0905 <S**2>=0.000
228 ->251 0.11149
236 ->251 0.28180
237 ->250 0.33562
237 ->251 0.45553
240 ->250 -0.12996
240 ->251 0.11344

Excited State 42: Singlet-E 3.2551 eV 380.89 nm f=0.0905 <S**2>=0.000
228 ->250 0.11149
236 ->250 0.28180
237 ->250 0.45553
237 ->251 -0.33562
240 ->250 -0.11344
240 ->251 -0.12996

Excited State 43: Singlet-E 3.3235 eV 373.06 nm f=0.0004 <S**2>=0.000
227 ->250 0.43183
227 ->251 0.40572
228 ->250 0.11843
232 ->250 0.14942
232 ->251 0.15357
235 ->250 -0.11991

Excited State 44: Singlet-E 3.3235 eV 373.06 nm f=0.0004 <S**2>=0.000
227 ->250 -0.40572
227 ->251 0.43183
228 ->251 0.11843
232 ->250 -0.15357
232 ->251 0.14942
235 ->251 0.11991

Excited state symmetry could not be determined.
Excited State 45: Singlet-?Sym 3.3275 eV 372.61 nm f=0.0012 <S**2>=0.000

232 ->252 0.10857
233 ->250 0.30915
233 ->255 -0.12006
234 ->251 0.30915
234 ->254 0.12006
235 ->253 0.12696
241 ->260 0.10800
242 ->257 0.15607
243 ->259 0.13055
244 ->258 -0.13055
245 ->256 0.15548
246 ->254 0.14380
247 ->255 0.14380
248 ->253 0.14637
249 ->252 0.11720

Excited state symmetry could not be determined.
Excited State 46: Singlet-?Sym 3.3305 eV 372.27 nm f=0.0000 <S**2>=0.000
232 ->253 0.10923
233 ->250 -0.30072
233 ->255 0.11880
234 ->251 0.30072
234 ->254 0.11880
235 ->252 0.12059
235 ->260 0.10224
241 ->253 0.12297
242 ->256 0.15574
243 ->259 0.15086
244 ->258 0.15086
245 ->257 0.15508
246 ->254 0.14840
247 ->255 -0.14840
248 ->252 0.11492
248 ->260 0.13510
249 ->253 0.10319

Excited State 47: Singlet-E 3.3355 eV 371.71 nm f=0.0142 <S**2>=0.000
227 ->250 0.16136
227 ->251 0.24238
228 ->251 0.11737
232 ->251 -0.20540
235 ->250 0.24481
235 ->251 -0.14115
236 ->250 -0.11479
237 ->250 0.11199

237 ->251 0.11795
242 ->258 0.12618
243 ->257 -0.10782
244 ->256 0.11275
245 ->259 -0.12408

Excited State 48: Singlet-E 3.3355 eV 371.71 nm f=0.0142 <S**2>=0.000
227 ->250 0.24238
227 ->251 -0.16136
228 ->250 0.11737
232 ->250 -0.20540
235 ->250 0.14115
235 ->251 0.24481
236 ->251 0.11479
237 ->250 0.11795
237 ->251 -0.11199
242 ->259 0.12618
243 ->256 0.11275
244 ->257 -0.10782
245 ->258 -0.12408

Excited State 49: Singlet-B 3.5378 eV 350.45 nm f=0.0000 <S**2>=0.000
232 ->256 0.22389
233 ->258 0.24317
234 ->259 0.24317
235 ->257 0.26114
236 ->256 0.13348
242 ->253 0.14970
243 ->254 0.14566
244 ->255 0.14566
245 ->252 0.13497
245 ->260 0.13269
246 ->259 -0.14316
247 ->258 0.14316
248 ->257 -0.15770
249 ->256 -0.14292

Excited State 50: Singlet-A 3.5380 eV 350.44 nm f=0.0000 <S**2>=0.000
232 ->257 0.22410
233 ->258 -0.23185
233 ->259 -0.11353
234 ->258 -0.11353
234 ->259 0.23185
235 ->256 0.26106
236 ->257 0.13356

242 ->252 0.13470
242 ->260 0.13317
243 ->254 0.14358
244 ->255 -0.14358
245 ->253 0.14906
246 ->259 -0.14139
247 ->258 -0.14139
248 ->256 -0.15776
249 ->257 -0.14273

Excited State 51: Singlet-E 3.5381 eV 350.43 nm f=0.0003 <S**2>=0.000
232 ->258 -0.18003
232 ->259 0.12992
233 ->256 -0.14788
233 ->257 0.12264
234 ->256 0.21441
234 ->257 0.22995
235 ->259 0.25585
236 ->258 -0.10714
242 ->254 0.12401
243 ->252 0.12463
243 ->253 0.11400
243 ->260 0.12334
245 ->254 0.12766
246 ->256 -0.13285
246 ->257 -0.13310
248 ->259 -0.15456
249 ->258 0.11545

Excited State 52: Singlet-E 3.5381 eV 350.43 nm f=0.0003 <S**2>=0.000
232 ->258 -0.12992
232 ->259 -0.18003
233 ->256 -0.21441
233 ->257 0.22995
234 ->256 -0.14788
234 ->257 -0.12264
235 ->258 0.25585
236 ->259 -0.10714
242 ->255 -0.12401
244 ->252 0.12463
244 ->253 -0.11400
244 ->260 0.12334
245 ->255 0.12766
247 ->256 -0.13285
247 ->257 0.13310

248 ->258 -0.15456
249 ->259 0.11545

Excited state symmetry could not be determined.
Excited State 53: Singlet-?Sym 3.6210 eV 342.41 nm f=0.0000 <S**2>=0.000
230 ->250 0.46800
231 ->251 -0.46800

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 3.6220 eV 342.31 nm f=0.0000 <S**2>=0.000
230 ->250 0.44652
230 ->251 0.17327
231 ->250 -0.17327
231 ->251 0.44652

Excited State 55: Singlet-E 3.6282 eV 341.72 nm f=0.0290 <S**2>=0.000
227 ->250 -0.11535
228 ->250 0.21600
228 ->251 -0.25089
229 ->250 0.14719
229 ->251 0.44085
232 ->250 0.12351
236 ->250 -0.29013
236 ->251 0.13985
237 ->251 -0.10696

Excited State 56: Singlet-E 3.6282 eV 341.72 nm f=0.0290 <S**2>=0.000
227 ->251 -0.11535
228 ->250 0.25089
228 ->251 0.21600
229 ->250 0.44085
229 ->251 -0.14719
232 ->251 0.12351
236 ->250 -0.13985
236 ->251 -0.29013
237 ->250 0.10696

Excited state symmetry could not be determined.
Excited State 57: Singlet-?Sym 3.6621 eV 338.56 nm f=0.0005 <S**2>=0.000
233 ->251 -0.46354
234 ->250 0.46354

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 3.6664 eV 338.16 nm f=0.0000 <S**2>=0.000
233 ->250 -0.10579

233 ->251 0.47716
234 ->250 0.47716
234 ->251 0.10579

Excited State 59: Singlet-E 3.6676 eV 338.05 nm f=0.0048 <S**2>=0.000
232 ->250 -0.24033
232 ->251 -0.33902
235 ->250 -0.40721
235 ->251 0.28324
236 ->250 -0.14373
236 ->251 -0.20411

Excited State 60: Singlet-E 3.6676 eV 338.05 nm f=0.0048 <S**2>=0.000
232 ->250 0.33902
232 ->251 -0.24033
235 ->250 0.28324
235 ->251 0.40721
236 ->250 0.20411
236 ->251 -0.14373

Excited State 61: Singlet-B 3.7062 eV 334.53 nm f=0.0170 <S**2>=0.000
221 ->250 0.11855
222 ->251 0.11855
230 ->251 -0.31763
231 ->250 -0.31763
249 ->252 0.44113

Excited State 62: Singlet-B 3.7137 eV 333.86 nm f=0.0548 <S**2>=0.000
217 ->250 0.15197
218 ->251 -0.15197
221 ->250 -0.12676
221 ->251 -0.11181
222 ->250 0.11181
222 ->251 -0.12676
230 ->251 0.20065
231 ->250 0.20065
233 ->251 -0.11538
234 ->250 0.11538
249 ->252 0.48793

Excited state symmetry could not be determined.
Excited State 63: Singlet-?Sym 3.7195 eV 333.34 nm f=0.0000 <S**2>=0.000
221 ->251 -0.11525
222 ->250 -0.11525
230 ->250 0.14842

230 ->251 -0.44058
231 ->250 0.44058
231 ->251 0.14842

Excited State 64: Singlet-E 3.7245 eV 332.88 nm f=0.1356 <S**2>=0.000
227 ->250 0.11603
228 ->250 -0.21848
228 ->251 0.12148
229 ->250 0.34402
229 ->251 0.38648
232 ->250 -0.20946
236 ->250 0.28180
237 ->250 -0.11367

Excited State 65: Singlet-E 3.7245 eV 332.88 nm f=0.1356 <S**2>=0.000
227 ->251 0.11603
228 ->250 -0.12148
228 ->251 -0.21848
229 ->250 0.38648
229 ->251 -0.34402
232 ->251 -0.20946
236 ->251 0.28180
237 ->251 -0.11367

Excited state symmetry could not be determined.
Excited State 66: Singlet-?Sym 3.7453 eV 331.04 nm f=0.0029 <S**2>=0.000
217 ->250 -0.22383
218 ->251 0.22383
221 ->251 0.20390
222 ->250 -0.20390
227 ->252 0.10934
230 ->250 -0.11078
230 ->251 0.28519
231 ->250 0.28519
231 ->251 0.11078
233 ->250 0.11454
234 ->251 0.11454
249 ->252 0.14631

Excited state symmetry could not be determined.
Excited State 67: Singlet-?Sym 3.7476 eV 330.84 nm f=0.0000 <S**2>=0.000
217 ->250 0.24387
218 ->251 0.24387
221 ->250 -0.10530
221 ->251 0.22069

222 ->250 0.22069
222 ->251 0.10530
230 ->250 0.10248
230 ->251 -0.11179
231 ->250 0.11179
231 ->251 0.10248
232 ->253 -0.11562
233 ->250 -0.22705
233 ->255 -0.13075
234 ->251 0.22705
234 ->254 -0.13075
235 ->260 -0.13038

Excited State 68: Singlet-E 3.7647 eV 329.33 nm f=0.0009 <S**2>=0.000
232 ->250 0.15816
232 ->251 0.27187
232 ->254 -0.14030
232 ->255 0.10723
233 ->253 0.13167
233 ->260 -0.11204
234 ->253 -0.15764
234 ->260 -0.17007
235 ->250 -0.23100
235 ->251 0.24724
235 ->254 -0.16609
235 ->255 -0.11990
236 ->251 0.13394

Excited State 69: Singlet-E 3.7647 eV 329.33 nm f=0.0009 <S**2>=0.000
232 ->250 0.27187
232 ->251 -0.15816
232 ->254 0.10723
232 ->255 0.14030
233 ->253 0.15764
233 ->260 -0.17007
234 ->253 0.13167
234 ->260 0.11204
235 ->250 -0.24724
235 ->251 -0.23100
235 ->254 0.11990
235 ->255 -0.16609
236 ->250 0.13394

Excited state symmetry could not be determined.
Excited State 70: Singlet-?Sym 3.7669 eV 329.14 nm f=0.0006 <S**2>=0.000

230 ->251 -0.10251
231 ->250 -0.10251
232 ->260 -0.15909
233 ->250 0.31449
233 ->255 0.18594
234 ->251 0.31449
234 ->254 -0.18594
235 ->253 -0.18801

Excited state symmetry could not be determined.
Excited State 71: Singlet-?Sym 3.7764 eV 328.32 nm f=0.0000 <S**2>=0.000
217 ->250 -0.21428
218 ->251 -0.21428
221 ->251 -0.18980
222 ->250 -0.18980
232 ->253 -0.13291
233 ->250 -0.24770
233 ->255 -0.15472
234 ->251 0.24770
234 ->254 -0.15472
235 ->260 -0.15501

Excited state symmetry could not be determined.
Excited State 72: Singlet-?Sym 3.8462 eV 322.36 nm f=0.0001 <S**2>=0.000
217 ->250 0.11337
217 ->251 0.31109
218 ->250 0.31109
218 ->251 -0.11337
221 ->250 0.25060
221 ->251 -0.22586
222 ->250 0.22586
222 ->251 0.25060
230 ->251 0.10600
231 ->250 0.10600

Excited state symmetry could not be determined.
Excited State 73: Singlet-?Sym 3.8517 eV 321.89 nm f=0.0000 <S**2>=0.000
217 ->251 -0.33435
218 ->250 0.33435
221 ->250 0.30837
221 ->251 0.12558
222 ->250 0.12558
222 ->251 -0.30837
230 ->251 -0.10771
231 ->250 0.10771

Excited State 74: Singlet-E 3.8576 eV 321.40 nm f=0.9685 <S**2>=0.000
223 ->250 -0.11343
228 ->250 0.30405
228 ->251 -0.36656
232 ->250 -0.12757
236 ->250 0.25966
237 ->251 0.27055
246 ->252 0.10100

Excited State 75: Singlet-E 3.8576 eV 321.40 nm f=0.9685 <S**2>=0.000
223 ->251 -0.11343
228 ->250 0.36656
228 ->251 0.30405
232 ->251 -0.12757
236 ->251 0.25966
237 ->250 -0.27055
247 ->252 0.10100

Excited state symmetry could not be determined.
Excited State 76: Singlet-?Sym 4.0013 eV 309.86 nm f=0.0000 <S**2>=0.000
224 ->250 0.43754
224 ->251 0.17254
225 ->250 -0.17254
225 ->251 0.43754
248 ->252 0.10676

Excited state symmetry could not be determined.
Excited State 77: Singlet-?Sym 4.0044 eV 309.62 nm f=0.0146 <S**2>=0.000
224 ->250 0.46146
224 ->251 0.13321
225 ->250 0.13321
225 ->251 -0.46146

Excited State 78: Singlet-E 4.0162 eV 308.71 nm f=0.0502 <S**2>=0.000
223 ->250 -0.33958
226 ->250 0.33551
226 ->251 0.45061
246 ->252 -0.10568

Excited State 79: Singlet-E 4.0162 eV 308.71 nm f=0.0502 <S**2>=0.000
223 ->251 -0.33958
226 ->250 0.45061
226 ->251 -0.33551
247 ->252 -0.10568

Excited State 80: Singlet-A 4.0556 eV 305.71 nm f=0.0000 <S**2>=0.000
248 ->252 0.64799
248 ->260 -0.11476

Excited State 81: Singlet-E 4.0891 eV 303.21 nm f=0.0652 <S**2>=0.000
226 ->251 -0.14361
247 ->252 0.61532
247 ->260 -0.10526

Excited State 82: Singlet-E 4.0891 eV 303.21 nm f=0.0652 <S**2>=0.000
226 ->250 0.14361
246 ->252 0.61532
246 ->260 -0.10526

Excited state symmetry could not be determined.
Excited State 83: Singlet-?Sym 4.1079 eV 301.82 nm f=0.0001 <S**2>=0.000
224 ->250 -0.13364
224 ->251 0.45801
225 ->250 0.45801
225 ->251 0.13364
245 ->252 0.15211

Excited state symmetry could not be determined.
Excited State 84: Singlet-?Sym 4.1110 eV 301.59 nm f=0.0000 <S**2>=0.000
224 ->250 0.16673
224 ->251 -0.43241
225 ->250 0.43241
225 ->251 0.16673
242 ->252 0.19759

Excited State 85: Singlet-E 4.1179 eV 301.08 nm f=0.0446 <S**2>=0.000
223 ->250 0.19545
223 ->251 -0.49949
226 ->251 0.32142
244 ->252 -0.23931

Excited State 86: Singlet-E 4.1179 eV 301.08 nm f=0.0446 <S**2>=0.000
223 ->250 0.49949
223 ->251 0.19545
226 ->250 0.32142
243 ->252 0.23931

Excited State 87: Singlet-B 4.1198 eV 300.95 nm f=0.0001 <S**2>=0.000
224 ->251 -0.10571

225 ->250 -0.10571
245 ->252 0.63592
245 ->260 -0.11525

Excited State 88: Singlet-E 4.1247 eV 300.59 nm f=0.0053 <S**2>=0.000
219 ->251 0.10465
223 ->250 -0.22989
226 ->250 -0.12982
243 ->252 0.49491
244 ->252 -0.31467

Excited State 89: Singlet-E 4.1247 eV 300.59 nm f=0.0053 <S**2>=0.000
219 ->250 -0.10465
223 ->251 -0.22989
226 ->251 0.12982
243 ->252 0.31467
244 ->252 0.49491

Excited State 90: Singlet-A 4.1259 eV 300.50 nm f=0.0000 <S**2>=0.000
224 ->251 0.14046
225 ->250 -0.14046
242 ->252 0.61992
242 ->260 -0.11211

Excited State 91: Singlet-E 4.1626 eV 297.85 nm f=0.0203 <S**2>=0.000
219 ->250 -0.29793
219 ->251 0.32549
220 ->250 0.10426
220 ->251 0.48242
243 ->252 -0.14571

Excited State 92: Singlet-E 4.1626 eV 297.85 nm f=0.0203 <S**2>=0.000
219 ->250 -0.32548
219 ->251 -0.29793
220 ->250 0.48242
220 ->251 -0.10426
244 ->252 -0.14571

Excited state symmetry could not be determined.
Excited State 93: Singlet-?Sym 4.1792 eV 296.67 nm f=0.0003 <S**2>=0.000
217 ->250 -0.33843
218 ->251 0.33843
221 ->251 -0.32791
222 ->250 0.32791

Excited state symmetry could not be determined.
Excited State 94: Singlet-?Sym 4.1799 eV 296.62 nm f=0.0000 <S**2>=0.000
217 ->250 0.33481
218 ->251 0.33481
221 ->250 0.18828
221 ->251 -0.27133
222 ->250 -0.27133
222 ->251 -0.18828
242 ->252 0.10381

Excited State 95: Singlet-B 4.2319 eV 292.97 nm f=0.0033 <S**2>=0.000
241 ->252 0.66301

Excited State 96: Singlet-E 4.2885 eV 289.11 nm f=0.0010 <S**2>=0.000
219 ->250 0.43224
219 ->251 -0.26941
220 ->250 0.21570
220 ->251 0.41292

Excited State 97: Singlet-E 4.2885 eV 289.11 nm f=0.0010 <S**2>=0.000
219 ->250 0.26942
219 ->251 0.43225
220 ->250 0.41292
220 ->251 -0.21570

Excited state symmetry could not be determined.
Excited State 98: Singlet-?Sym 4.3107 eV 287.62 nm f=0.0000 <S**2>=0.000
217 ->251 -0.34160
218 ->250 0.34160
221 ->250 -0.28671
221 ->251 -0.20058
222 ->250 -0.20058
222 ->251 0.28671

Excited state symmetry could not be determined.
Excited State 99: Singlet-?Sym 4.3107 eV 287.62 nm f=0.0000 <S**2>=0.000
217 ->251 -0.34176
218 ->250 -0.34176
221 ->250 0.35435
222 ->251 0.35435

Excited State 100: Singlet-E 4.4264 eV 280.10 nm f=0.0011 <S**2>=0.000
212 ->251 -0.10765
213 ->250 -0.37851
213 ->251 0.55994

Table S8: Vertical Excitation energies of $TAP^{FcCN}Mg$ using PBE1PBE PCM-TDDFT

Excited State 1: Singlet-E 2.0978 eV 591.03 nm f=0.0074 <S**2>=0.000
266 ->274 -0.27795
266 ->275 -0.30415
266 ->278 -0.10053
267 ->277 -0.11154
268 ->276 -0.16496
269 ->274 0.29946
269 ->275 -0.29552
269 ->279 0.10196
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3455.58432332
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-E 2.0978 eV 591.03 nm f=0.0074 <S**2>=0.000
266 ->274 -0.30415
266 ->275 0.27795
266 ->279 -0.10053
267 ->276 -0.16496
268 ->277 -0.11154
269 ->274 0.29552
269 ->275 0.29946
269 ->278 0.10196

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 2.0987 eV 590.76 nm f=0.0001 <S**2>=0.000
266 ->277 0.12934
267 ->274 0.39813
267 ->275 0.12643
267 ->278 0.11811
268 ->274 0.12643
268 ->275 -0.39813
268 ->279 0.11811
269 ->276 -0.18998
269 ->280 0.10398

Excited state symmetry could not be determined.
Excited State 4: Singlet-?Sym 2.0987 eV 590.76 nm f=0.0000 <S**2>=0.000
266 ->276 0.18957
266 ->280 -0.10195
267 ->274 0.40443
267 ->275 -0.10348
267 ->278 0.10260

268 ->274 0.10348
268 ->275 0.40443
268 ->279 -0.10260
269 ->277 -0.12944

Excited State 5: Singlet-E 2.1150 eV 586.20 nm f=0.3548 <S**2>=0.000
265 ->274 0.10033
265 ->275 0.11712
270 ->276 -0.10881
272 ->274 -0.23783
272 ->275 0.19874
273 ->274 0.38274
273 ->275 0.33496

Excited State 6: Singlet-E 2.1150 eV 586.20 nm f=0.3548 <S**2>=0.000
265 ->274 -0.11712
265 ->275 0.10033
271 ->276 0.10881
272 ->274 0.19874
272 ->275 0.23783
273 ->274 -0.33496
273 ->275 0.38274

Excited state symmetry could not be determined.
Excited State 7: Singlet-?Sym 2.1730 eV 570.57 nm f=0.0390 <S**2>=0.000
265 ->276 0.10413
270 ->274 -0.41413
270 ->278 -0.10472
270 ->286 -0.10062
271 ->275 0.41413
271 ->279 -0.10472
271 ->287 -0.10062
272 ->277 -0.11527
272 ->285 -0.10690
273 ->276 0.13189

Excited state symmetry could not be determined.
Excited State 8: Singlet-?Sym 2.1970 eV 564.35 nm f=0.0000 <S**2>=0.000
270 ->274 0.41194
270 ->278 0.10498
270 ->286 0.10502
271 ->275 0.41194
271 ->279 -0.10498
271 ->287 -0.10502
272 ->276 0.15955

272 ->280 -0.10584

Excited State 9: Singlet-E 2.3616 eV 525.01 nm f=0.1064 <S**2>=0.000
272 ->274 0.20221
272 ->275 0.48715
273 ->274 0.16368
273 ->275 -0.39674

Excited State 10: Singlet-E 2.3616 eV 525.01 nm f=0.1064 <S**2>=0.000
272 ->274 0.48715
272 ->275 -0.20221
273 ->274 0.39674
273 ->275 0.16368

Excited state symmetry could not be determined.
Excited State 11: Singlet-?Sym 2.4668 eV 502.61 nm f=0.0000 <S**2>=0.000
270 ->275 -0.49642
271 ->274 0.49642

Excited state symmetry could not be determined.
Excited State 12: Singlet-?Sym 2.4736 eV 501.23 nm f=0.0002 <S**2>=0.000
270 ->275 0.49739
271 ->274 0.49739

Excited State 13: Singlet-E 2.5685 eV 482.71 nm f=0.0087 <S**2>=0.000
266 ->274 0.46926
266 ->275 -0.15775
269 ->274 0.46555
269 ->275 0.17666

Excited State 14: Singlet-E 2.5685 eV 482.71 nm f=0.0087 <S**2>=0.000
266 ->274 0.15775
266 ->275 0.46926
269 ->274 0.17666
269 ->275 -0.46555

Excited state symmetry could not be determined.
Excited State 15: Singlet-?Sym 2.5702 eV 482.39 nm f=0.0012 <S**2>=0.000
267 ->274 -0.14362
267 ->275 0.47426
268 ->274 0.47426
268 ->275 0.14362

Excited state symmetry could not be determined.
Excited State 16: Singlet-?Sym 2.5709 eV 482.26 nm f=0.0000 <S**2>=0.000

267 ->274 -0.12746
267 ->275 -0.48228
268 ->274 0.48228
268 ->275 -0.12746

Excited State 17: Singlet-E 2.6672 eV 464.84 nm f=0.3529 <S**2>=0.000
264 ->274 0.11179
265 ->274 0.41656
266 ->282 -0.14985
267 ->281 0.15369
267 ->284 0.11420
269 ->282 0.14558
272 ->274 0.29309
273 ->274 -0.15510

Excited State 18: Singlet-E 2.6672 eV 464.84 nm f=0.3529 <S**2>=0.000
264 ->275 -0.11179
265 ->275 0.41656
266 ->283 0.14985
268 ->281 0.15369
268 ->284 -0.11420
269 ->283 0.14558
272 ->275 -0.29309
273 ->275 -0.15510

Excited State 19: Singlet-B 2.7316 eV 453.88 nm f=0.0123 <S**2>=0.000
266 ->281 0.25334
267 ->282 -0.25258
268 ->283 0.25258
269 ->280 0.14250
269 ->284 -0.20825
270 ->274 0.20152
270 ->278 -0.10073
270 ->286 -0.10128
271 ->275 -0.20152
271 ->279 -0.10073
271 ->287 -0.10128
272 ->277 -0.10034
272 ->285 -0.10882

Excited State 20: Singlet-A 2.7418 eV 452.19 nm f=0.0000 <S**2>=0.000
266 ->280 0.15569
266 ->284 -0.20758
267 ->282 0.21435
267 ->283 -0.14468

268 ->282 0.14468
268 ->283 0.21435
269 ->281 0.25968
270 ->274 -0.20382
271 ->275 -0.20382

Excited State 21: Singlet-E 2.7661 eV 448.23 nm f=0.0025 <S**2>=0.000
265 ->275 0.10151
265 ->282 0.14816
266 ->274 -0.21923
266 ->278 0.10245
266 ->286 0.12122
267 ->277 0.10117
267 ->284 -0.13242
267 ->285 0.12409
269 ->274 0.19257
269 ->278 -0.11220
269 ->286 -0.12732
270 ->280 -0.15269
270 ->281 0.24268
270 ->284 0.17770
272 ->282 -0.22809
273 ->282 0.18887

Excited State 22: Singlet-E 2.7661 eV 448.23 nm f=0.0025 <S**2>=0.000
265 ->274 -0.10151
265 ->283 0.14816
266 ->275 0.21923
266 ->279 0.10245
266 ->287 0.12122
268 ->277 0.10117
268 ->284 0.13242
268 ->285 0.12409
269 ->275 0.19257
269 ->279 0.11220
269 ->287 0.12732
271 ->280 0.15269
271 ->281 0.24268
271 ->284 -0.17770
272 ->283 0.22809
273 ->283 0.18887

Excited state symmetry could not be determined.
Excited State 23: Singlet-?Sym 2.7679 eV 447.93 nm f=0.0000 <S**2>=0.000
265 ->281 0.16188

266 ->280 0.12920
266 ->284 0.10346
267 ->274 0.20623
267 ->278 -0.10136
267 ->286 -0.13609
268 ->275 0.20623
268 ->279 0.10136
268 ->287 0.13609
269 ->277 0.11244
269 ->285 0.13778
270 ->282 0.23537
271 ->283 0.23537
272 ->280 0.15368
272 ->284 -0.19888
273 ->281 0.20826

Excited State 24: Singlet-B 2.7682 eV 447.89 nm f=0.0000 <S**2>=0.000
265 ->284 -0.13469
266 ->277 0.11265
266 ->285 0.13822
267 ->274 -0.20834
267 ->278 0.11443
267 ->286 0.11422
268 ->275 0.20834
268 ->279 0.11443
268 ->287 0.11422
269 ->280 0.14079
270 ->282 -0.24024
271 ->283 0.24024
272 ->281 0.25208
273 ->280 0.12120
273 ->284 -0.16870

Excited State 25: Singlet-E 2.7887 eV 444.59 nm f=0.0999 <S**2>=0.000
265 ->274 -0.14013
265 ->275 0.44523
266 ->282 -0.12437
266 ->283 -0.15285
267 ->281 0.12465
268 ->280 -0.13299
268 ->281 -0.16329
268 ->284 0.14477
269 ->283 -0.20678

Excited State 26: Singlet-E 2.7887 eV 444.59 nm f=0.0999 <S**2>=0.000

265 ->274 0.44523
265 ->275 0.14013
266 ->282 0.15285
266 ->283 -0.12437
267 ->280 0.13299
267 ->281 -0.16329
267 ->284 -0.14477
268 ->281 -0.12465
269 ->282 -0.20678

Excited state symmetry could not be determined.
Excited State 27: Singlet-?Sym 2.8467 eV 435.54 nm f=0.0000 <S**2>=0.000
253 ->276 0.12234
253 ->280 -0.11043
254 ->274 0.20726
254 ->275 -0.12420
254 ->286 0.13073
255 ->274 0.12420
255 ->275 0.20726
255 ->287 -0.13073
256 ->277 -0.14614
256 ->285 -0.13887
270 ->274 -0.15703
270 ->278 0.10993
270 ->286 0.11112
271 ->275 0.15703
271 ->279 0.10993
271 ->287 0.11112
272 ->277 0.11340
272 ->285 0.12183
273 ->276 -0.14343
273 ->280 0.10837

Excited state symmetry could not be determined.
Excited State 28: Singlet-?Sym 2.8541 eV 434.40 nm f=0.0000 <S**2>=0.000
253 ->277 -0.11408
253 ->285 -0.10765
254 ->274 -0.20025
254 ->275 -0.13471
254 ->278 -0.12965
254 ->287 0.10032
255 ->274 -0.13471
255 ->275 0.20025
255 ->279 -0.12965
255 ->286 -0.10032

256 ->276 0.15236
256 ->280 -0.13769
256 ->284 -0.10437
270 ->274 0.16400
270 ->278 -0.11378
270 ->286 -0.12122
271 ->275 0.16400
271 ->279 0.11378
271 ->287 0.12122
272 ->276 -0.10210
272 ->280 0.12286
272 ->284 0.10194
273 ->277 0.11716
273 ->285 0.11927

Excited State 29: Singlet-E 2.8560 eV 434.12 nm f=0.0033 <S**2>=0.000
253 ->275 0.18812
253 ->279 -0.10753
254 ->276 -0.10109
255 ->276 0.11249
255 ->277 -0.13176
255 ->280 -0.10154
255 ->285 -0.12472
256 ->275 0.23980
256 ->279 -0.12569
256 ->287 -0.13289
257 ->275 0.13903
265 ->275 0.16063
271 ->277 0.11569
271 ->280 0.12140
271 ->284 0.10097
271 ->285 0.12673
272 ->275 0.15557
272 ->279 0.11158
272 ->287 0.12680
273 ->275 0.10043
273 ->279 0.11544
273 ->287 0.10712

Excited State 30: Singlet-E 2.8560 eV 434.12 nm f=0.0033 <S**2>=0.000
253 ->274 -0.18812
253 ->278 -0.10753
254 ->276 -0.11249
254 ->277 -0.13176
254 ->280 0.10154

254 ->285 -0.12472
255 ->276 -0.10109
256 ->274 0.23980
256 ->278 0.12569
256 ->286 0.13289
257 ->274 -0.13903
265 ->274 -0.16063
270 ->277 -0.11569
270 ->280 0.12140
270 ->284 0.10097
270 ->285 -0.12673
272 ->274 0.15557
272 ->278 -0.11158
272 ->286 -0.12680
273 ->274 -0.10043
273 ->278 0.11544
273 ->286 0.10712

Excited state symmetry could not be determined.
Excited State 31: Singlet-?Sym 3.0116 eV 411.69 nm f=0.0344 <S**2>=0.000
262 ->274 -0.47189
263 ->275 0.47189

Excited State 32: Singlet-E 3.0167 eV 411.00 nm f=0.0534 <S**2>=0.000
264 ->274 0.53099
264 ->275 0.41030

Excited State 33: Singlet-E 3.0167 eV 411.00 nm f=0.0534 <S**2>=0.000
264 ->274 0.41030
264 ->275 -0.53099

Excited state symmetry could not be determined.
Excited State 34: Singlet-?Sym 3.0440 eV 407.31 nm f=0.0000 <S**2>=0.000
262 ->274 0.47177
263 ->275 0.47177

Excited State 35: Singlet-B 3.0484 eV 406.72 nm f=0.0001 <S**2>=0.000
253 ->284 -0.12601
254 ->282 0.12659
254 ->283 -0.15385
255 ->282 0.15385
255 ->283 0.12659
256 ->281 0.20081
266 ->277 -0.13347
266 ->285 -0.14458

267 ->274 0.13570
267 ->278 -0.13406
267 ->286 -0.12028
268 ->275 -0.13570
268 ->279 -0.13406
268 ->287 -0.12028
269 ->276 0.12887
269 ->280 -0.13428
269 ->284 -0.11619
270 ->282 -0.15360
271 ->283 0.15360
272 ->281 0.15797

Excited state symmetry could not be determined.
Excited State 36: Singlet-?Sym 3.0487 eV 406.68 nm f=0.0000 <S**2>=0.000
253 ->281 0.15909
254 ->282 -0.19344
255 ->283 0.19344
256 ->280 0.12006
256 ->284 -0.16058
257 ->281 0.11629
265 ->281 0.13260
266 ->276 0.12878
266 ->280 -0.14066
266 ->284 -0.10935
267 ->274 -0.13692
267 ->278 0.11621
267 ->286 0.14096
268 ->275 -0.13692
268 ->279 -0.11621
268 ->287 -0.14096
269 ->277 -0.13359
269 ->285 -0.14474
270 ->282 0.14770
271 ->283 0.14770
272 ->284 -0.12365
273 ->281 0.11348

Excited State 37: Singlet-E 3.0489 eV 406.65 nm f=0.0008 <S**2>=0.000
253 ->283 0.13681
254 ->281 -0.13905
255 ->280 0.11093
255 ->281 0.14323
255 ->284 -0.14968
256 ->283 0.19873

257 ->283 0.10020
265 ->283 0.11523
266 ->275 -0.13795
266 ->279 -0.13375
266 ->287 -0.12483
268 ->276 0.11419
268 ->277 -0.13253
268 ->280 -0.12803
268 ->285 -0.14353
269 ->275 -0.13745
269 ->279 -0.11979
269 ->287 -0.13990
271 ->281 0.15779
271 ->284 -0.11931
272 ->283 0.15679

Excited State 38: Singlet-E 3.0489 eV 406.65 nm f=0.0008 <S**2>=0.000
253 ->282 -0.13681
254 ->280 -0.11093
254 ->281 0.14323
254 ->284 0.14968
255 ->281 0.13905
256 ->282 0.19873
257 ->282 -0.10021
265 ->282 -0.11523
266 ->274 -0.13795
266 ->278 0.13375
266 ->286 0.12483
267 ->276 0.11419
267 ->277 0.13253
267 ->280 -0.12803
267 ->285 0.14353
269 ->274 0.13745
269 ->278 -0.11979
269 ->286 -0.13990
270 ->281 -0.15779
270 ->284 -0.11931
272 ->282 0.15679

Excited state symmetry could not be determined.
Excited State 39: Singlet-?Sym 3.1365 eV 395.29 nm f=0.0000 <S**2>=0.000
262 ->275 -0.49512
263 ->274 0.49512

Excited state symmetry could not be determined.

Excited State 40: Singlet-?Sym 3.1375 eV 395.17 nm f=0.0007 <S**2>=0.000
262 ->275 0.49540
263 ->274 0.49540

Excited State 41: Singlet-B 3.3651 eV 368.45 nm f=0.0338 <S**2>=0.000
254 ->274 0.25599
254 ->275 -0.14982
255 ->274 0.14982
255 ->275 0.25599
266 ->281 -0.14407
267 ->282 0.14293
268 ->283 -0.14293
269 ->284 0.10961
273 ->276 0.43686

Excited State 42: Singlet-E 3.3851 eV 366.26 nm f=0.0583 <S**2>=0.000
252 ->274 -0.14685
253 ->275 0.13382
256 ->275 0.22062
257 ->274 -0.14245
257 ->275 0.16255
261 ->274 -0.11617
261 ->275 0.41755
266 ->283 -0.11401
268 ->281 -0.11641
268 ->284 0.10146
269 ->283 -0.12490
271 ->276 0.18093

Excited State 43: Singlet-E 3.3851 eV 366.26 nm f=0.0583 <S**2>=0.000
252 ->275 0.14685
253 ->274 0.13382
256 ->274 -0.22062
257 ->274 0.16255
257 ->275 0.14245
261 ->274 0.41755
261 ->275 0.11617
266 ->282 0.11401
267 ->281 -0.11641
267 ->284 -0.10146
269 ->282 -0.12490
270 ->276 -0.18093

Excited state symmetry could not be determined.
Excited State 44: Singlet-?Sym 3.4064 eV 363.97 nm f=0.0000 <S**2>=0.000

254 ->274 -0.28152
254 ->275 -0.19306
255 ->274 -0.19306
255 ->275 0.28152
266 ->284 0.12926
267 ->282 -0.13512
268 ->283 -0.13512
269 ->281 -0.16292
272 ->276 0.24371

Excited State 45: Singlet-E 3.4252 eV 361.97 nm f=0.0621 <S**2>=0.000
252 ->275 0.16810
253 ->274 -0.22206
253 ->275 -0.13356
256 ->274 0.24888
257 ->274 -0.14866
257 ->275 0.13883
260 ->274 -0.15034
261 ->274 0.37553
261 ->275 0.10276
269 ->282 0.10379
270 ->276 0.15375

Excited State 46: Singlet-E 3.4252 eV 361.97 nm f=0.0621 <S**2>=0.000
252 ->274 -0.16810
253 ->274 0.13356
253 ->275 -0.22206
256 ->275 -0.24888
257 ->274 -0.13883
257 ->275 -0.14866
260 ->275 0.15034
261 ->274 -0.10276
261 ->275 0.37553
269 ->283 0.10379
271 ->276 -0.15375

Excited state symmetry could not be determined.
Excited State 47: Singlet-?Sym 3.4675 eV 357.56 nm f=0.0000 <S**2>=0.000
258 ->274 0.44234
258 ->275 0.21693
259 ->274 -0.21693
259 ->275 0.44234
260 ->276 0.10073

Excited state symmetry could not be determined.

Excited State 48: Singlet-?Sym 3.4677 eV 357.54 nm f=0.0000 <S**2>=0.000
258 ->274 -0.45560
258 ->275 0.18708
259 ->274 0.18708
259 ->275 0.45560

Excited State 49: Singlet-E 3.4753 eV 356.76 nm f=0.0224 <S**2>=0.000
247 ->274 0.10624
252 ->275 0.13927
253 ->274 -0.26057
257 ->274 0.37831
260 ->274 0.43047
260 ->275 0.12088
261 ->275 0.16692

Excited State 50: Singlet-E 3.4753 eV 356.76 nm f=0.0224 <S**2>=0.000
247 ->275 -0.10624
252 ->274 0.13927
253 ->275 0.26057
257 ->275 -0.37831
260 ->274 -0.12088
260 ->275 0.43047
261 ->274 0.16692

Excited State 51: Singlet-B 3.5423 eV 350.01 nm f=0.0568 <S**2>=0.000
254 ->274 -0.16805
254 ->275 0.11297
255 ->274 -0.11297
255 ->275 -0.16805
265 ->276 -0.12978
270 ->286 0.11282
271 ->287 0.11282
272 ->277 0.10561
272 ->285 0.11994
273 ->276 0.49998
273 ->280 0.10405

Excited State 52: Singlet-E 3.5556 eV 348.70 nm f=0.0026 <S**2>=0.000
243 ->274 0.13675
243 ->275 0.10921
247 ->274 0.39877
247 ->275 0.31683
248 ->274 0.25632
248 ->275 0.20422
260 ->274 -0.20855

260 ->275 0.12269

Excited State 53: Singlet-E 3.5556 eV 348.70 nm f=0.0026 <S**2>=0.000
243 ->274 0.10921
243 ->275 -0.13675
247 ->274 0.31683
247 ->275 -0.39877
248 ->274 0.20422
248 ->275 -0.25632
260 ->274 -0.12269
260 ->275 -0.20855

Excited state symmetry could not be determined.
Excited State 54: Singlet-?Sym 3.6004 eV 344.37 nm f=0.0000 <S**2>=0.000
258 ->274 0.21743
258 ->275 -0.44132
259 ->274 0.44132
259 ->275 0.21743

Excited state symmetry could not be determined.
Excited State 55: Singlet-?Sym 3.6005 eV 344.35 nm f=0.0040 <S**2>=0.000
258 ->274 0.18621
258 ->275 0.44747
259 ->274 0.44747
259 ->275 -0.18621

Excited State 56: Singlet-E 3.6007 eV 344.34 nm f=0.0300 <S**2>=0.000
256 ->274 0.25138
256 ->275 -0.12345
257 ->274 0.42477
257 ->275 0.13750
260 ->274 -0.39505
261 ->274 -0.18376

Excited State 57: Singlet-E 3.6007 eV 344.34 nm f=0.0300 <S**2>=0.000
256 ->274 0.12345
256 ->275 0.25138
257 ->274 0.13750
257 ->275 -0.42477
260 ->275 -0.39505
261 ->275 0.18376

Excited state symmetry could not be determined.
Excited State 58: Singlet-?Sym 3.6094 eV 343.51 nm f=0.0000 <S**2>=0.000
254 ->274 -0.24891

254 ->275 -0.41793
255 ->274 0.41793
255 ->275 -0.24891

Excited state symmetry could not be determined.
Excited State 59: Singlet-?Sym 3.6098 eV 343.46 nm f=0.0000 <S**2>=0.000
254 ->274 -0.27145
254 ->275 0.40857
255 ->274 0.40857
255 ->275 0.27145

Excited State 60: Singlet-E 3.6186 eV 342.63 nm f=0.0004 <S**2>=0.000
247 ->275 0.17526
248 ->275 0.14124
253 ->275 0.45171
256 ->275 -0.38867
260 ->275 -0.21205
261 ->275 0.13663

Excited State 61: Singlet-E 3.6186 eV 342.63 nm f=0.0004 <S**2>=0.000
247 ->274 0.17526
248 ->274 0.14124
253 ->274 0.45171
256 ->274 0.38867
260 ->274 0.21205
261 ->274 0.13663

Excited State 62: Singlet-A 3.7367 eV 331.80 nm f=0.0000 <S**2>=0.000
254 ->274 0.12946
255 ->275 -0.12946
256 ->280 -0.10475
266 ->276 0.24206
272 ->276 0.54252

Excited State 63: Singlet-B 3.7376 eV 331.72 nm f=0.0001 <S**2>=0.000
254 ->283 0.11253
255 ->282 -0.11253
256 ->281 -0.14759
269 ->276 0.59645

Excited State 64: Singlet-E 3.7383 eV 331.66 nm f=0.0075 <S**2>=0.000
254 ->281 0.10383
256 ->283 -0.12305
267 ->276 -0.31245
268 ->276 0.39229

270 ->276 -0.32068

Excited State 65: Singlet-E 3.7383 eV 331.66 nm f=0.0075 <S**2>=0.000
255 ->281 -0.10383
256 ->282 -0.12305
267 ->276 0.39229
268 ->276 0.31245
271 ->276 0.32068

Excited State 66: Singlet-A 3.7411 eV 331.41 nm f=0.0000 <S**2>=0.000
253 ->281 -0.10602
254 ->282 0.13152
255 ->283 -0.13152
256 ->284 0.13327
266 ->276 0.54353
272 ->276 -0.24155

Excited State 67: Singlet-E 3.7463 eV 330.95 nm f=0.0092 <S**2>=0.000
253 ->275 -0.10851
256 ->275 -0.14296
267 ->276 -0.17781
268 ->276 -0.26830
270 ->276 -0.16253
271 ->276 0.46476

Excited State 68: Singlet-E 3.7463 eV 330.95 nm f=0.0092 <S**2>=0.000
253 ->274 0.10851
256 ->274 -0.14296
267 ->276 -0.26830
268 ->276 0.17782
270 ->276 0.46476
271 ->276 0.16253

Excited state symmetry could not be determined.
Excited State 69: Singlet-?Sym 3.8523 eV 321.85 nm f=0.0017 <S**2>=0.000
249 ->274 0.37989
250 ->275 -0.37989
256 ->285 -0.10161
265 ->276 0.24587

Excited State 70: Singlet-E 3.8637 eV 320.90 nm f=0.0219 <S**2>=0.000
247 ->275 -0.22331
248 ->275 0.34294
251 ->275 0.50237
271 ->276 0.11388

Excited State 71: Singlet-E 3.8637 eV 320.90 nm f=0.0219 <S**2>=0.000
247 ->274 0.22331
248 ->274 -0.34294
251 ->274 0.50237
270 ->276 0.11388

Excited state symmetry could not be determined.
Excited State 72: Singlet-?Sym 3.8642 eV 320.85 nm f=0.0000 <S**2>=0.000
249 ->274 0.44517
249 ->275 0.14121
250 ->274 -0.14121
250 ->275 0.44517
272 ->276 0.11071

Excited State 73: Singlet-B 3.8970 eV 318.16 nm f=0.0058 <S**2>=0.000
241 ->274 -0.13492
241 ->275 -0.11594
242 ->274 0.11594
242 ->275 -0.13492
245 ->274 0.22154
246 ->275 -0.22154
249 ->274 -0.19604
250 ->275 0.19604
265 ->276 0.34716

Excited State 74: Singlet-B 3.9098 eV 317.11 nm f=0.0135 <S**2>=0.000
241 ->274 0.11320
242 ->275 0.11320
245 ->274 -0.26011
246 ->275 0.26011
247 ->276 -0.10432
249 ->274 -0.19755
250 ->275 0.19755
265 ->276 0.29303
269 ->276 0.14513

Excited state symmetry could not be determined.
Excited State 75: Singlet-?Sym 3.9156 eV 316.64 nm f=0.0000 <S**2>=0.000
241 ->275 0.15760
242 ->274 0.15760
245 ->274 0.35834
246 ->275 0.35834
253 ->281 0.10017
254 ->282 -0.12070

255 ->283 0.12070
266 ->276 0.20383

Excited State 76: Singlet-E 3.9383 eV 314.81 nm f=0.0200 <S**2>=0.000
243 ->274 -0.26587
244 ->274 0.28972
253 ->282 -0.13654
254 ->281 0.16132
255 ->284 0.10204
256 ->282 0.14946
257 ->282 -0.10167
266 ->286 -0.10796
267 ->276 0.24680
267 ->280 0.10144
273 ->282 0.10748

Excited State 77: Singlet-E 3.9383 eV 314.81 nm f=0.0200 <S**2>=0.000
243 ->275 0.26587
244 ->275 0.28972
253 ->283 0.13654
254 ->284 0.10204
255 ->281 0.16132
256 ->283 0.14946
257 ->283 0.10167
266 ->287 0.10796
268 ->276 0.24680
268 ->280 0.10144
273 ->283 -0.10748

Excited state symmetry could not be determined.
Excited State 78: Singlet-?Sym 3.9801 eV 311.51 nm f=0.0042 <S**2>=0.000
241 ->274 0.27443
241 ->275 0.16075
242 ->274 -0.16075
242 ->275 0.27443
245 ->275 0.10012
246 ->274 0.10012
247 ->276 -0.11352
254 ->283 0.11832
255 ->282 -0.11832
256 ->281 -0.15459
269 ->276 -0.18820

Excited state symmetry could not be determined.
Excited State 79: Singlet-?Sym 3.9884 eV 310.86 nm f=0.0000 <S**2>=0.000

241 ->275 0.22522
242 ->274 0.22522
249 ->274 -0.12287
249 ->275 0.11787
250 ->274 -0.11787
250 ->275 -0.12287
254 ->282 0.11925
255 ->283 -0.11925
256 ->284 0.16906
266 ->276 -0.14067
266 ->284 -0.11968
272 ->276 0.10297
272 ->280 0.11021

Excited State 80: Singlet-E 3.9908 eV 310.68 nm f=0.2427 <S**2>=0.000
251 ->275 0.21234
252 ->274 -0.21893
253 ->287 -0.10660
255 ->280 -0.12682
255 ->285 -0.11083
256 ->275 -0.17260
256 ->279 -0.12375
256 ->287 -0.12612
257 ->275 -0.12823
263 ->276 -0.12365
266 ->283 -0.10713
268 ->281 -0.10937
269 ->283 -0.10560
271 ->276 -0.12383

Excited State 81: Singlet-E 3.9908 eV 310.68 nm f=0.2427 <S**2>=0.000
251 ->274 0.21234
252 ->275 -0.21893
253 ->286 -0.10660
254 ->280 0.12682
254 ->285 -0.11083
256 ->274 -0.17260
256 ->278 0.12375
256 ->286 0.12612
257 ->274 0.12823
262 ->276 -0.12365
266 ->282 -0.10713
267 ->281 0.10937
269 ->282 0.10560
270 ->276 -0.12383

Excited state symmetry could not be determined.
Excited State 82: Singlet-?Sym 4.0036 eV 309.68 nm f=0.0000 <S**2>=0.000
241 ->275 -0.15351
242 ->274 -0.15351
249 ->275 -0.23800
250 ->274 0.23800
254 ->274 -0.12171
254 ->278 0.10012
255 ->275 0.12171
255 ->279 0.10012
256 ->280 0.15694
272 ->276 0.11947

Excited state symmetry could not be determined.
Excited State 83: Singlet-?Sym 4.0108 eV 309.13 nm f=0.0002 <S**2>=0.000
249 ->274 0.10930
249 ->275 0.47430
250 ->274 0.47430
250 ->275 -0.10930

Excited State 84: Singlet-E 4.0200 eV 308.42 nm f=0.0109 <S**2>=0.000
247 ->275 -0.28652
248 ->274 -0.11647
248 ->275 0.44356
251 ->275 -0.41739

Excited State 85: Singlet-E 4.0200 eV 308.42 nm f=0.0109 <S**2>=0.000
247 ->274 -0.28652
248 ->274 0.44356
248 ->275 0.11647
251 ->274 0.41739

Excited state symmetry could not be determined.
Excited State 86: Singlet-?Sym 4.0216 eV 308.30 nm f=0.0000 <S**2>=0.000
241 ->275 0.11976
242 ->274 0.11976
249 ->274 0.15446
249 ->275 -0.39135
250 ->274 0.39135
250 ->275 0.15446

Excited State 87: Singlet-E 4.0490 eV 306.21 nm f=0.7417 <S**2>=0.000
243 ->274 -0.11402
244 ->274 0.11470

252 ->274 0.31432
252 ->275 0.37420
253 ->274 0.11686
261 ->274 -0.15096

Excited State 88: Singlet-E 4.0490 eV 306.21 nm f=0.7417 <S**2>=0.000
243 ->275 0.11402
244 ->275 0.11470
252 ->274 0.37420
252 ->275 -0.31432
253 ->275 -0.11686
261 ->275 0.15096

Excited state symmetry could not be determined.
Excited State 89: Singlet-?Sym 4.0575 eV 305.57 nm f=0.0002 <S**2>=0.000
241 ->274 0.22869
241 ->275 -0.15232
242 ->274 0.15232
242 ->275 0.22869
245 ->274 0.20608
245 ->275 0.22497
246 ->274 0.22497
246 ->275 -0.20608
265 ->276 -0.19291

Excited State 90: Singlet-B 4.0601 eV 305.37 nm f=0.0004 <S**2>=0.000
245 ->274 0.15269
246 ->275 -0.15269
253 ->280 0.11249
254 ->274 0.10320
254 ->286 -0.11030
255 ->275 0.10320
255 ->287 0.11030
256 ->277 0.10624
256 ->285 0.11616
265 ->276 0.37487

Excited state symmetry could not be determined.
Excited State 91: Singlet-?Sym 4.0773 eV 304.08 nm f=0.0000 <S**2>=0.000
241 ->274 0.29575
241 ->275 0.19335
242 ->274 0.19335
242 ->275 -0.29575
245 ->275 -0.32918
246 ->274 0.32918

Excited State 92: Singlet-E 4.0831 eV 303.65 nm f=0.2603 <S**2>=0.000
243 ->274 -0.32080
244 ->274 0.40606
252 ->274 -0.18204
252 ->275 -0.10777
256 ->282 -0.10768

Excited State 93: Singlet-E 4.0831 eV 303.65 nm f=0.2603 <S**2>=0.000
243 ->275 0.32080
244 ->275 0.40606
252 ->274 -0.10777
252 ->275 0.18204
256 ->283 -0.10768

Excited state symmetry could not be determined.
Excited State 94: Singlet-?Sym 4.1232 eV 300.70 nm f=0.0000 <S**2>=0.000
241 ->274 0.22823
241 ->275 -0.27106
242 ->274 -0.27106
242 ->275 -0.22823
245 ->274 0.28318
246 ->275 0.28318

Excited state symmetry could not be determined.
Excited State 95: Singlet-?Sym 4.1299 eV 300.21 nm f=0.0002 <S**2>=0.000
241 ->275 -0.35268
242 ->274 0.35268
245 ->274 -0.23108
245 ->275 0.18468
246 ->274 0.18468
246 ->275 0.23108

Excited State 96: Singlet-E 4.2072 eV 294.69 nm f=0.0084 <S**2>=0.000
243 ->274 0.12158
243 ->275 -0.48550
244 ->275 0.45920
247 ->275 0.14599

Excited State 97: Singlet-E 4.2072 eV 294.69 nm f=0.0084 <S**2>=0.000
243 ->274 0.48550
243 ->275 0.12158
244 ->274 0.45920
247 ->274 -0.14599

Excited state symmetry could not be determined.
Excited State 98: Singlet-?Sym 4.2487 eV 291.81 nm f=0.0000 <S**2>=0.000
241 ->274 -0.24033
241 ->275 0.20298
242 ->274 -0.20298
242 ->275 -0.24033
245 ->275 0.38391
246 ->274 0.38391

Excited state symmetry could not be determined.
Excited State 99: Singlet-?Sym 4.2542 eV 291.44 nm f=0.0000 <S**2>=0.000
241 ->274 -0.30465
241 ->275 -0.13659
242 ->274 -0.13659
242 ->275 0.30465
245 ->275 -0.36665
246 ->274 0.36665

Excited State 100: Singlet-A 4.3268 eV 286.55 nm f=0.0000 <S**2>=0.000
264 ->276 0.68172

Table S9: Molecular Orbital Composition Raw Data from TAP^{Fc}Mg B3LYP single point calculation

Orbital	HOMO/LUMO	Energy (eV)	% Mg	% Por	% Fe	% Cp
230.00	-19	-6.993	0.00	3.08	6.98	89.93
231.00	-18	-6.993	0.00	3.08	7.08	89.83
232.00	-17	-6.942	0.20	49.50	15.73	34.57
233.00	-16	-6.916	0.01	4.85	84.87	10.27
234.00	-15	-6.916	0.01	4.85	84.56	10.58
235.00	-14	-6.915	0.00	2.80	88.10	9.10
236.00	-13	-6.912	0.03	12.66	74.85	12.45
237.00	-12	-6.685	0.04	58.82	7.08	34.07
238.00	-11	-6.412	0.00	38.88	13.26	47.86
239.00	-10	-6.412	0.00	38.88	13.65	47.48
240.00	-9	-6.352	0.00	40.09	15.05	44.87
241.00	-8	-6.001	0.00	33.86	43.63	22.50
242.00	-7	-5.832	0.00	0.60	85.25	14.15
243.00	-6	-5.832	0.00	0.50	85.14	14.36
244.00	-5	-5.832	0.00	0.50	85.47	14.03
245.00	-4	-5.827	0.00	0.78	85.16	14.06
246.00	-3	-5.765	0.01	7.61	78.34	14.04
247.00	-2	-5.765	0.01	7.61	78.45	13.92
248.00	-1	-5.747	0.00	8.52	77.53	13.94
249.00	0	-5.527	0.03	38.05	45.63	16.29
250.00	0	-3.337	0.00	90.78	4.65	4.58
251.00	1	-3.337	0.00	90.78	4.65	4.56
252.00	2	-1.892	0.00	78.67	10.72	10.60
253.00	3	-0.724	0.11	11.60	50.95	37.34
254.00	4	-0.703	0.17	14.27	51.26	34.31
255.00	5	-0.703	0.17	14.27	47.51	38.05
256.00	6	-0.624	0.04	1.01	54.20	44.76
257.00	7	-0.620	0.00	0.45	54.35	45.19
258.00	8	-0.619	0.03	0.70	54.47	44.80
259.00	9	-0.619	0.03	0.70	54.21	45.06
260.00	10	-0.552	0.06	14.29	45.16	40.48
261.00	11	0.261	11.94	15.70	59.82	12.53
262.00	12	0.266	0.75	14.08	59.99	25.18
263.00	13	0.270	0.17	34.52	29.94	35.37

264.00	14	0.270	0.17	34.52	29.88	35.42
265.00	15	0.307	0.22	6.62	73.40	19.76
266.00	16	0.398	0.02	83.64	1.84	14.50
267.00	17	0.425	0.06	10.75	69.00	20.18
268.00	18	0.425	0.06	10.75	69.23	19.96
269.00	19	0.495	3.82	19.17	46.01	30.99

Table S10: Molecular Orbital Composition Raw Data from TAP^{FcCN}Mg B3LYP single point calculation

Orbital	HOMO/LUMO	Energy (eV)	% Mg	% Por	% Fe	% Cp
254	-19	-7.181	0.01	5.63	56.64	37.72
255	-18	-7.181	0.01	5.63	56.64	37.72
256	-17	-7.18	0.00	3.94	49.20	46.86
257	-16	-7.179	0.00	2.83	39.39	57.78
258	-15	-7.179	0.00	2.83	39.39	57.78
259	-14	-7.179	0.00	2.90	49.76	47.34
260	-13	-7.175	0.00	6.04	68.24	25.72
261	-12	-7.118	0.01	41.82	14.84	43.32
262	-11	-6.788	0.00	38.09	12.54	49.37
263	-10	-6.788	0.00	38.09	12.54	49.37
264	-9	-6.741	0.00	39.37	12.64	47.98
265	-8	-6.373	0.01	36.27	30.94	32.78
266	-7	-6.116	0.00	0.63	85.80	13.56
267	-6	-6.116	0.00	0.68	85.70	13.62
268	-5	-6.116	0.00	0.68	85.70	13.62
269	-4	-6.113	0.00	0.71	85.68	13.60
270	-3	-6.04	0.00	8.48	76.94	14.58
271	-2	-6.04	0.00	8.48	76.94	14.58
272	-1	-6.024	0.00	7.71	77.78	14.52
273	0	-5.831	0.02	24.88	57.44	17.66
274	0	-3.986	0.00	86.87	6.48	6.64
275	1	-3.986	0.00	86.87	6.48	6.64
276	2	-2.835	0.00	81.50	9.32	9.18
277	3	-1.336	0.03	60.34	21.92	17.70
278	4	-1.263	0.04	62.70	21.06	16.19
279	5	-1.263	0.04	62.70	21.06	16.19
280	6	-0.872	0.00	14.17	46.00	39.82
281	7	-0.858	0.00	1.16	53.76	45.08
282	8	-0.858	0.03	1.04	53.91	45.03

283	9	-0.858	0.03	1.04	53.91	45.03
284	10	-0.854	0.09	6.93	49.58	43.40
285	11	-0.675	0.51	32.19	28.70	38.60
286	12	-0.654	0.17	35.20	27.22	37.41
287	13	-0.654	0.17	35.20	27.22	37.41
288	14	-0.344	0.00	85.68	3.52	10.80
289	15	-0.083	4.29	72.13	11.54	12.04
290	16	-0.019	0.55	80.45	7.47	11.54
291	17	-0.019	0.55	80.45	7.47	11.54
292	18	0.04	0.03	83.29	6.76	9.90
293	19	0.127	11.02	37.84	36.58	14.56

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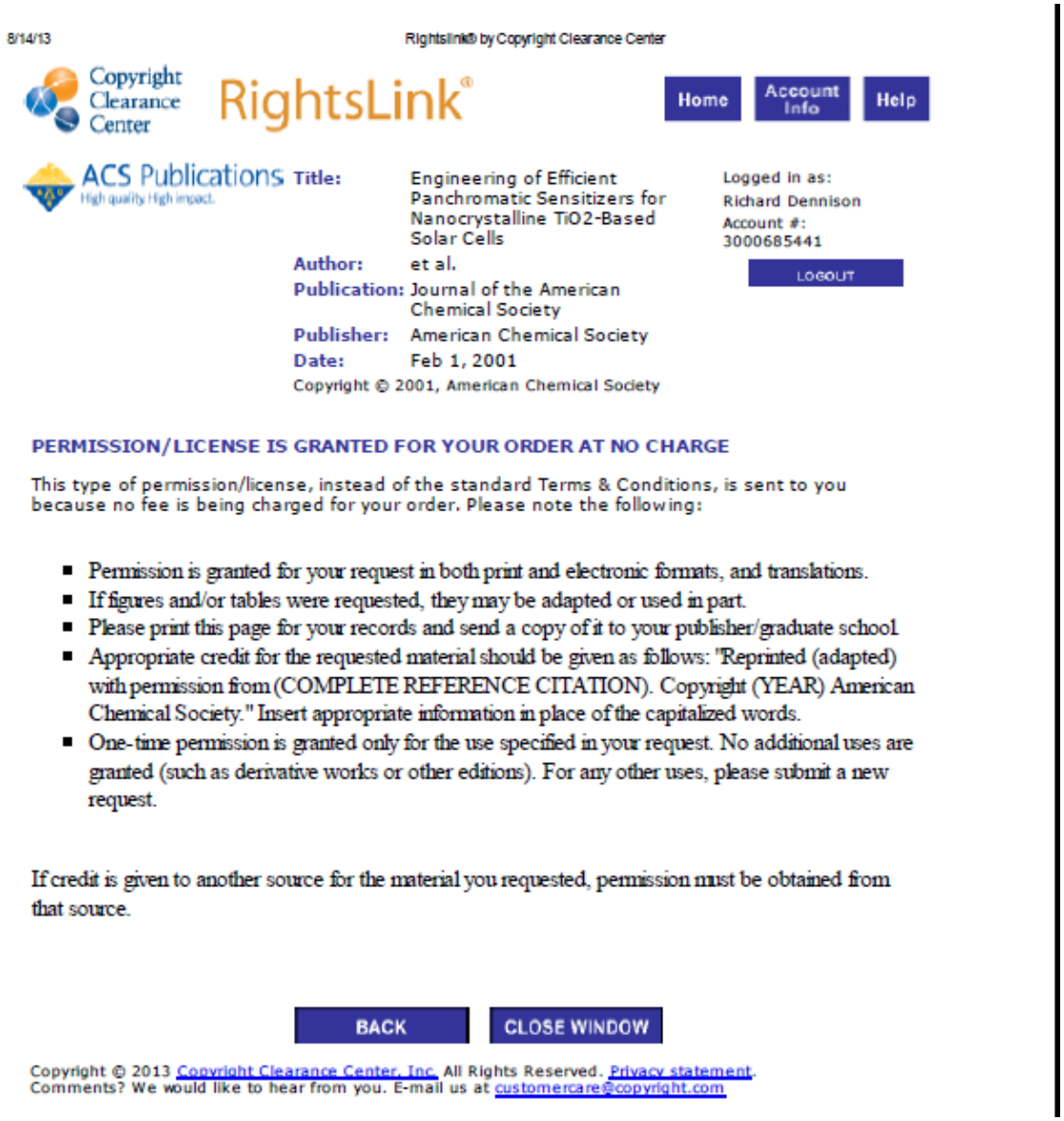

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